

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
 Data File : BF087982.D
 Acq On : 13 Jun 2016 14:37
 Operator : UM/SJ
 Sample : H3449-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 19-VE-PILE-WALL(0-2)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.724	11	12	22	rVV	298819	527091	17.70%	1.770%
2	1.861	22	24	37	rVV	1050426	2314504	77.72%	7.773%
3	2.021	37	38	55	rVB	67081	197209	6.62%	0.662%
4	4.296	235	237	240	rVB	21745	31382	1.05%	0.105%
5	4.970	293	296	305	rBB	157595	240664	8.08%	0.808%
6	5.393	330	333	335	rBV	2205899	2604507	87.46%	8.747%
7	6.433	421	424	426	rBV	2103474	2370798	79.61%	7.962%
8	6.559	432	435	438	rBV	2335896	2346802	78.81%	7.882%
9	6.787	453	455	458	rBV	698642	671583	22.55%	2.255%
10	6.947	466	469	472	rBV	2079926	1898538	63.75%	6.376%
11	7.359	502	505	507	rBV	1589843	1593285	53.50%	5.351%
12	8.079	565	568	570	rBV	1170142	966229	32.45%	3.245%
13	9.165	660	663	665	rBV	2872832	2977901	100.00%	10.001%
14	9.553	695	697	699	rVB	458883	367952	12.36%	1.236%
15	9.770	715	716	719	rBV	53064	47396	1.59%	0.159%
16	9.839	719	722	724	rBV	779365	1015921	34.12%	3.412%
17	10.273	758	760	762	rVB	108445	80569	2.71%	0.271%
18	10.491	776	779	782	rBV	32291	52138	1.75%	0.175%
19	10.616	788	790	793	rBV2	1171638	1622758	54.49%	5.450%
20	10.742	800	801	806	rVB	91875	105254	3.53%	0.353%
21	11.188	839	840	842	rBV	34603	40947	1.38%	0.138%
22	11.313	849	851	853	rBV	1121755	940836	31.59%	3.160%
23	11.565	869	873	875	rBV	17628	42181	1.42%	0.142%
24	11.851	896	898	902	rBV2	205713	257567	8.65%	0.865%
25	12.354	940	942	944	rBV	73140	59501	2.00%	0.200%
26	12.639	965	967	973	rBV	26245	44476	1.49%	0.149%
27	12.731	973	975	978	rVB	121076	115727	3.89%	0.389%
28	12.902	987	990	992	rBV	2184845	2076206	69.72%	6.973%
29	13.119	1007	1009	1013	rBV3	24760	55056	1.85%	0.185%
30	13.325	1026	1027	1029	rBV2	39447	57860	1.94%	0.194%
31	13.439	1035	1037	1039	rBV	60026	65239	2.19%	0.219%
32	13.817	1067	1070	1079	rBV	111218	273559	9.19%	0.919%
33	13.942	1079	1081	1084	rBV	749000	727365	24.43%	2.443%
34	14.457	1122	1126	1131	rBV2	72225	230537	7.74%	0.774%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.800	1153	1156	1158	rVB	74474	84700	2.84%	0.284%
36	14.868	1159	1162	1164	rVB	24210	36063	1.21%	0.121%
37	14.948	1167	1169	1174	rVB	16031	35572	1.19%	0.119%
38	15.051	1175	1178	1180	rBV	116366	165751	5.57%	0.557%
39	15.097	1180	1182	1190	rVB5	23033	68364	2.30%	0.230%
40	15.360	1202	1205	1207	rBV	503207	652377	21.91%	2.191%
41	15.405	1207	1209	1212	rVB	18375	31283	1.05%	0.105%
42	15.588	1222	1225	1228	rBV	58395	94527	3.17%	0.317%
43	15.805	1241	1244	1248	rBV	145709	225234	7.56%	0.756%
44	15.885	1248	1251	1253	rBV2	22906	52892	1.78%	0.178%
45	16.537	1306	1308	1313	rVB	33973	66606	2.24%	0.224%
46	16.765	1324	1328	1330	rBV	33836	73478	2.47%	0.247%
47	16.823	1330	1333	1335	rVV	31541	67318	2.26%	0.226%
48	16.880	1335	1338	1341	rVB	92562	165824	5.57%	0.557%
49	17.280	1369	1373	1383	rBV4	38320	157154	5.28%	0.528%
50	17.771	1413	1416	1420	rVB3	22942	52984	1.78%	0.178%
51	18.023	1434	1438	1449	rVV6	17987	89320	3.00%	0.300%
52	18.206	1450	1454	1463	rVB3	41869	129670	4.35%	0.435%
53	19.269	1540	1547	1563	rVB3	96135	507172	17.03%	1.703%

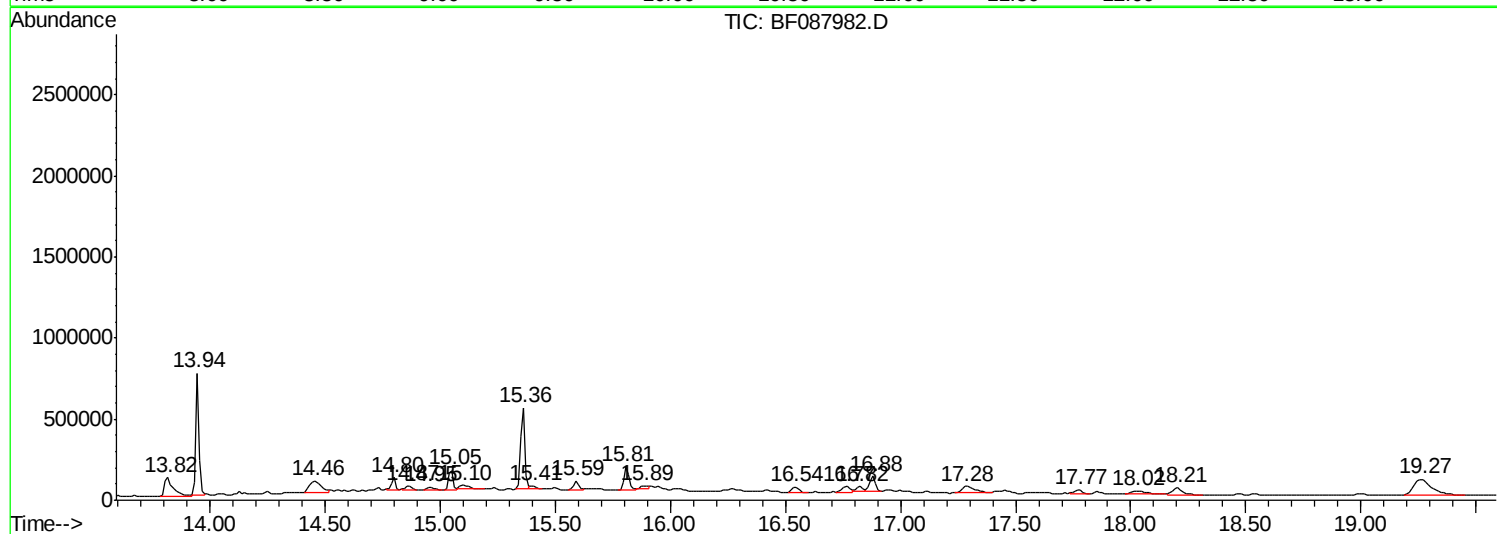
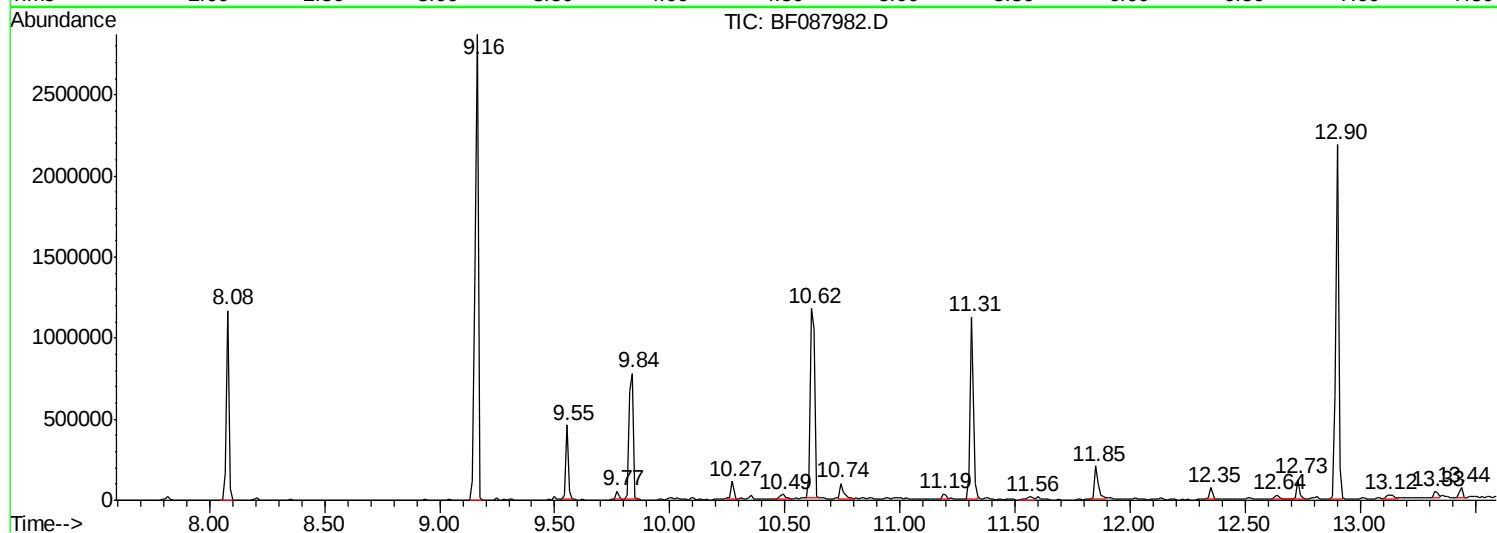
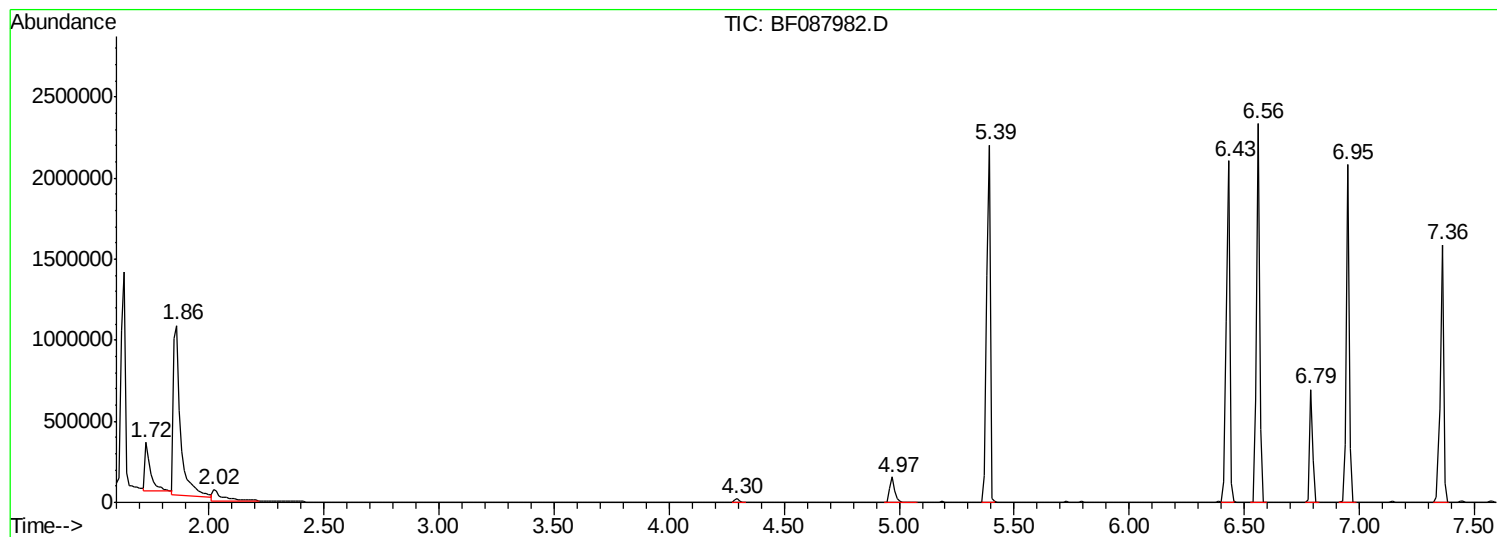
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Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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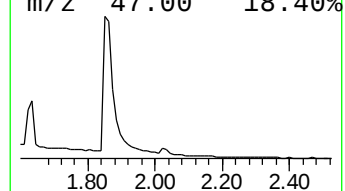
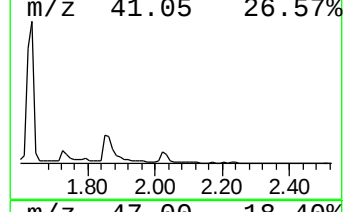
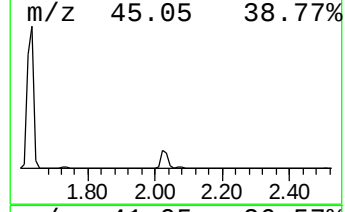
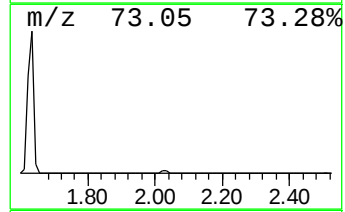
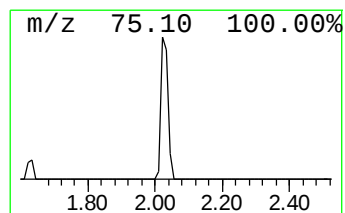
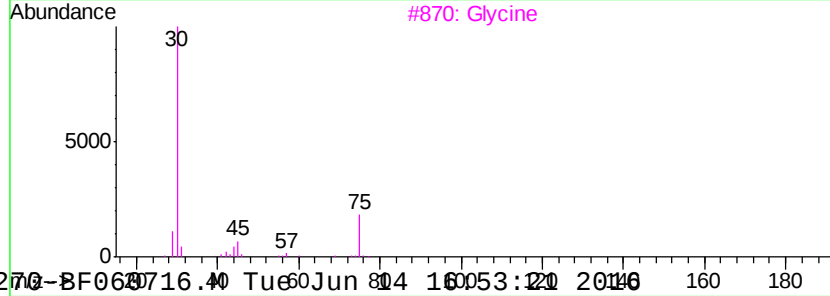
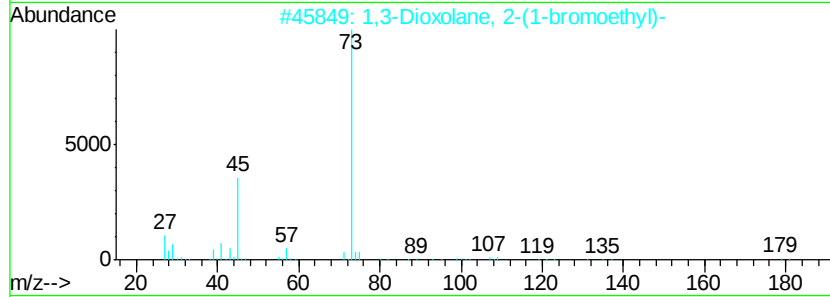
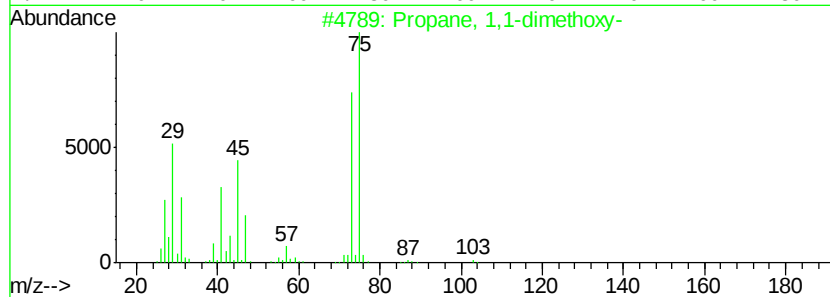
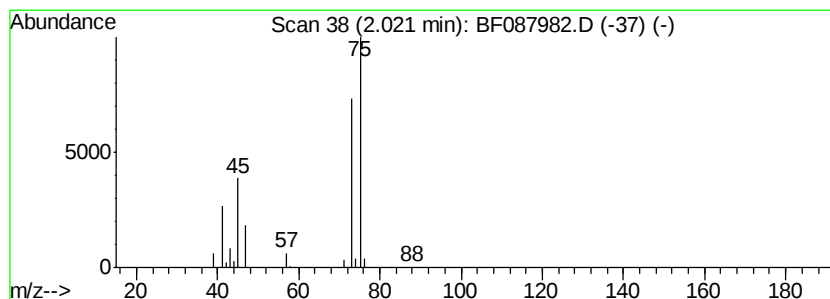
Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	5.87 ng	197209	1,4-Dichlorobenzene-d4	6.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
3		Glycine	75	C2H5NO2	000056-40-6	9
4		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9



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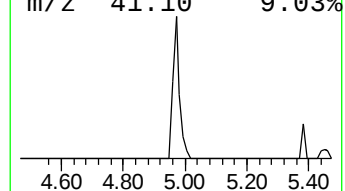
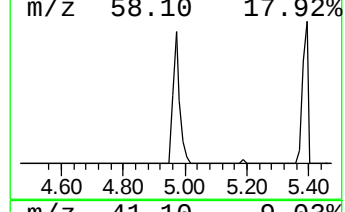
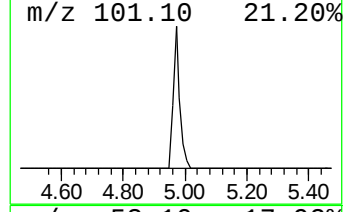
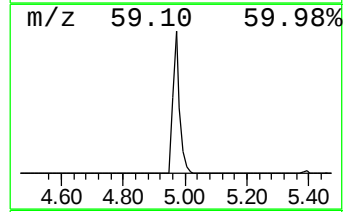
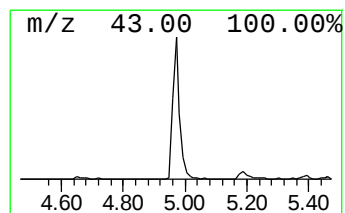
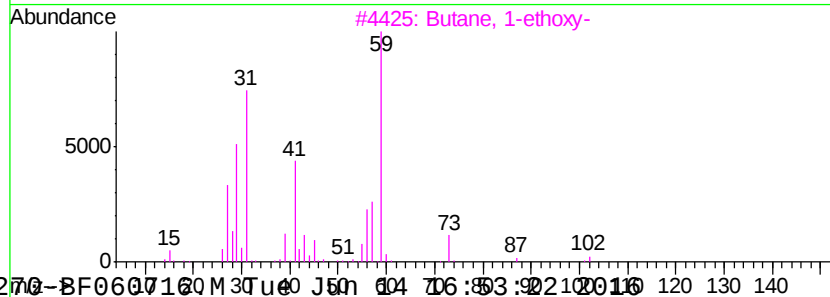
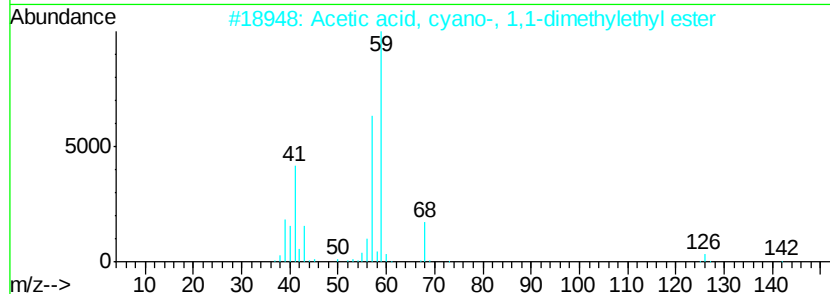
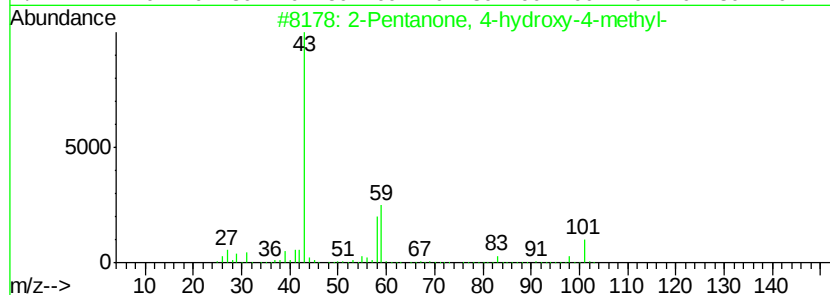
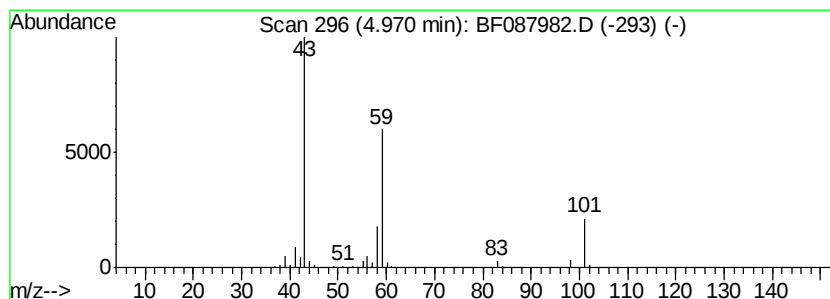
Instrument :
BNA_F
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19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.97	7.17 ng	240664	1,4-Dichlorobenzene-d4	6.79	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9



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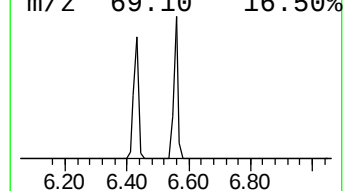
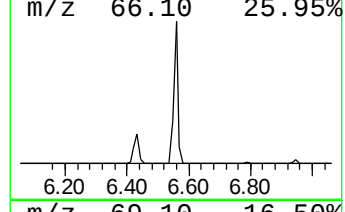
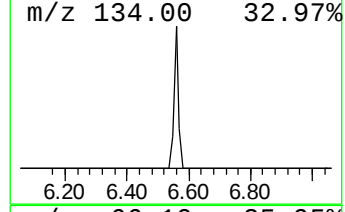
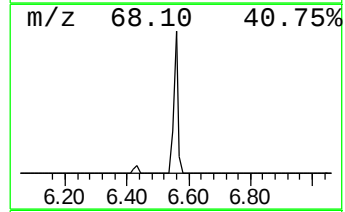
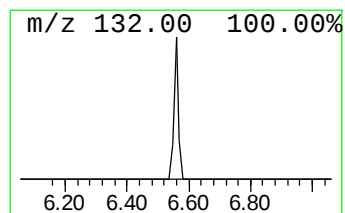
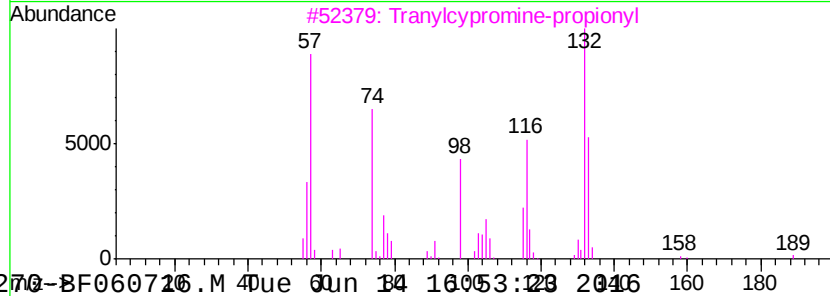
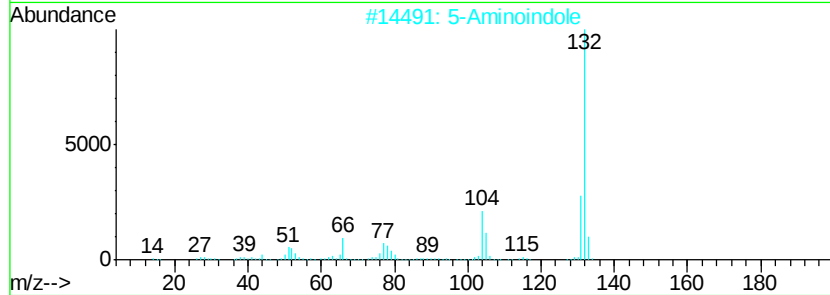
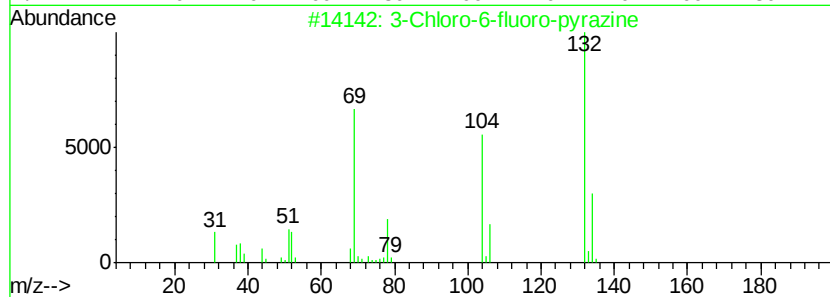
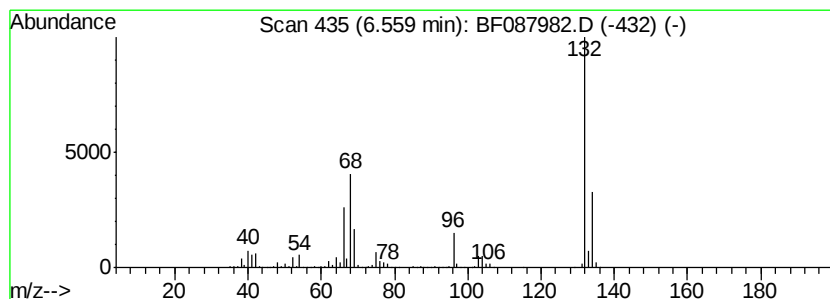
Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	69.89 ng	2346800	1,4-Dichlorobenzene-d4	6.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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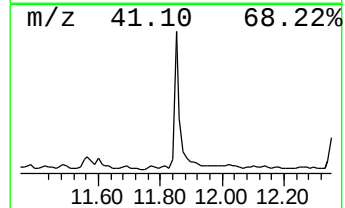
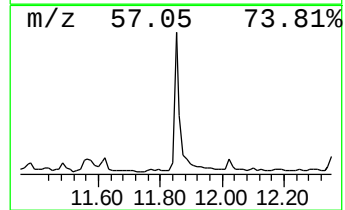
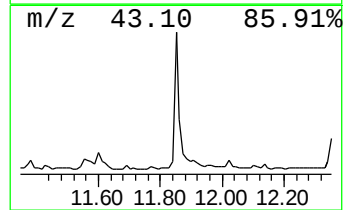
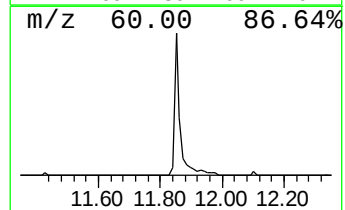
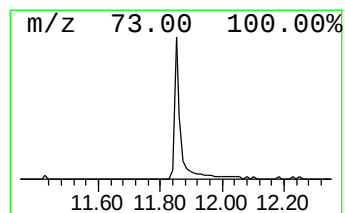
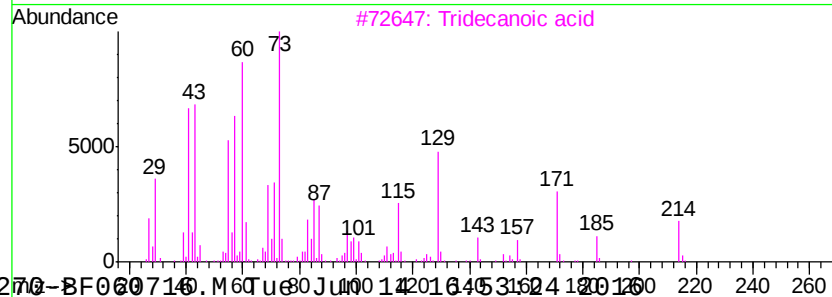
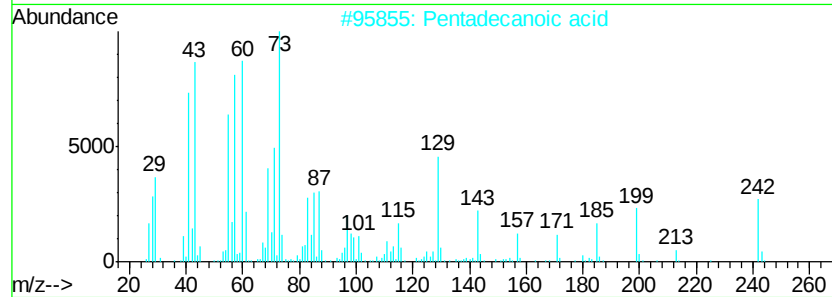
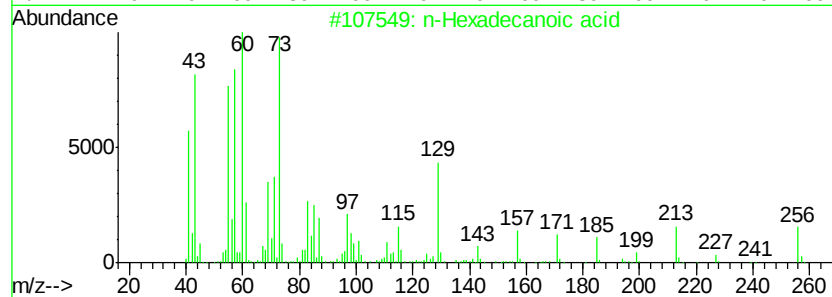
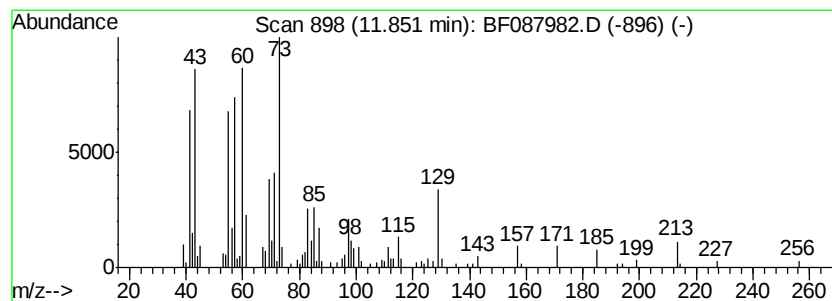
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	5.48 ng	257567	Phenanthrene-d10	11.31	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	35



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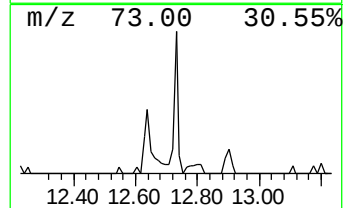
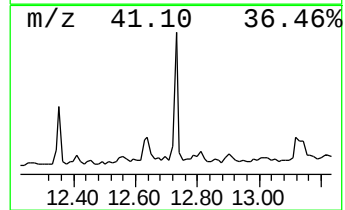
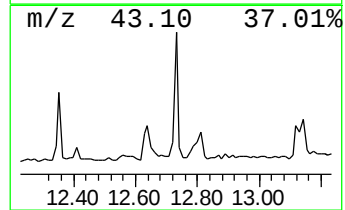
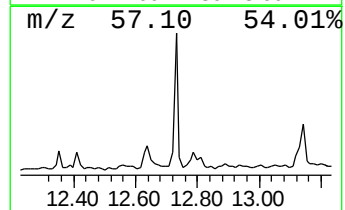
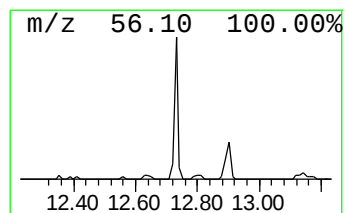
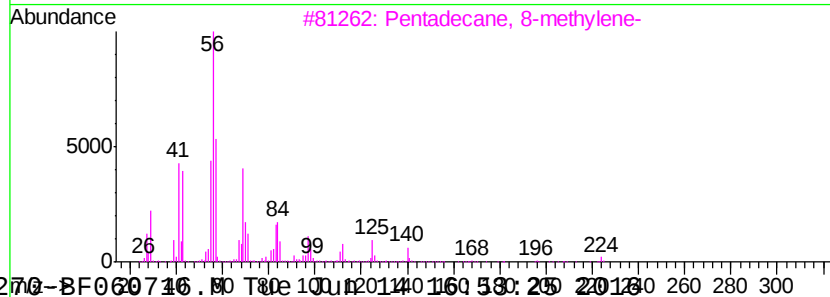
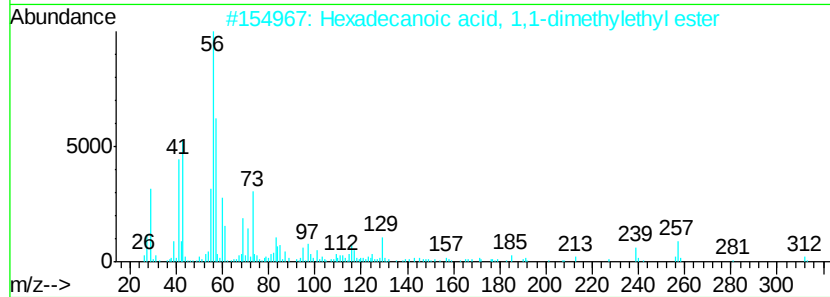
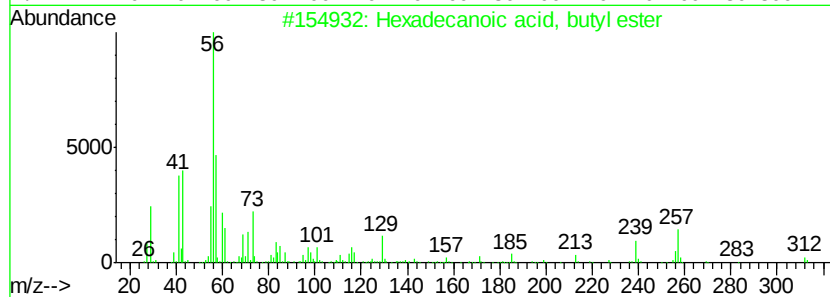
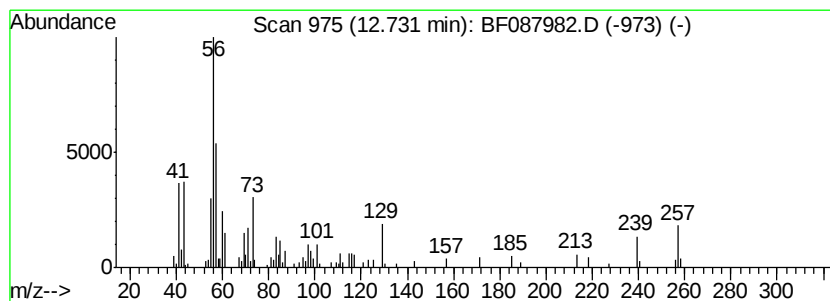
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ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.73	3.18 ng	115727	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	38
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

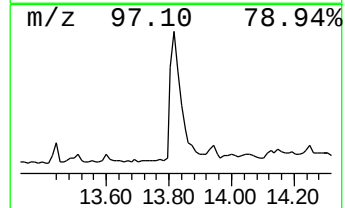
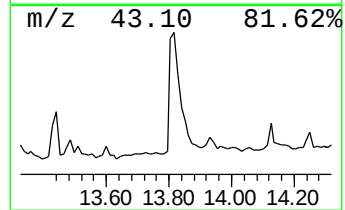
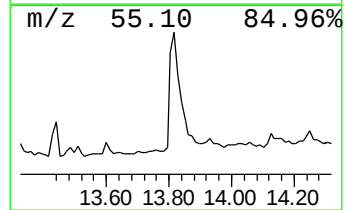
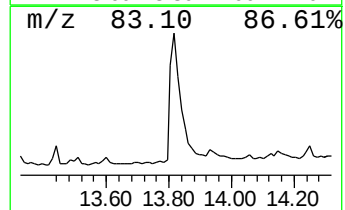
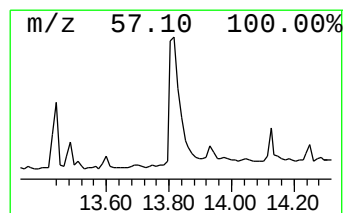
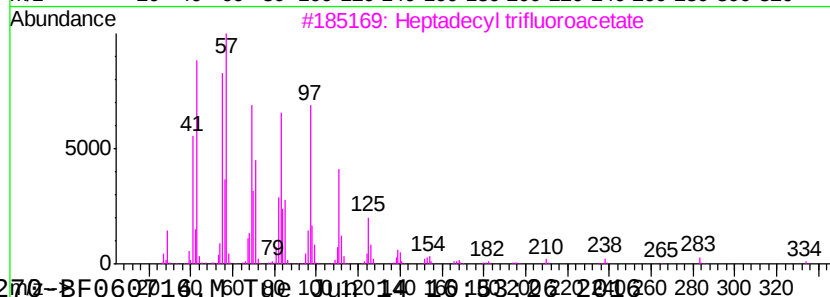
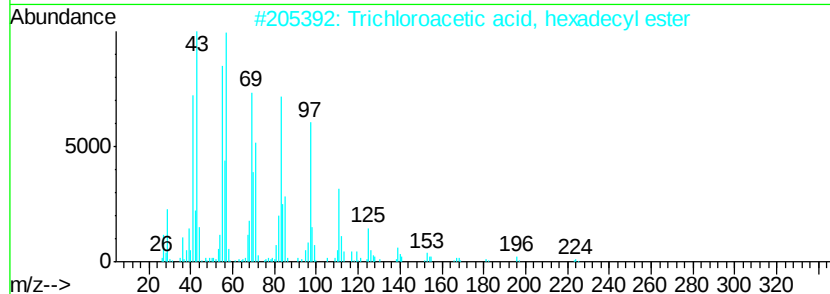
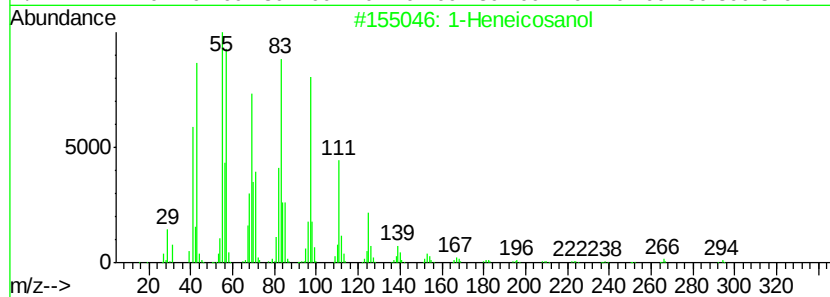
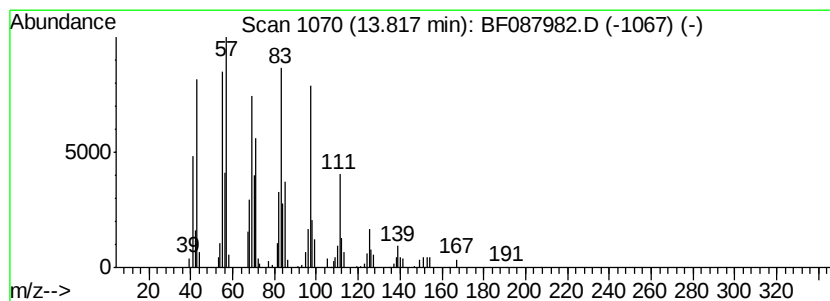
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ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	7.52 ng	273559	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	92
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
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Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

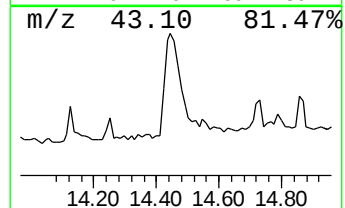
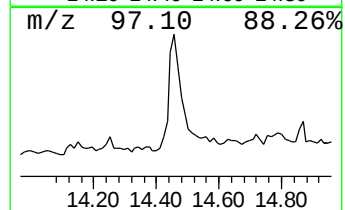
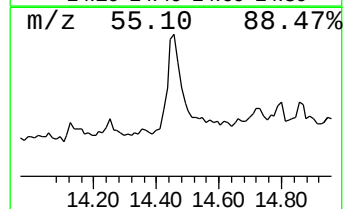
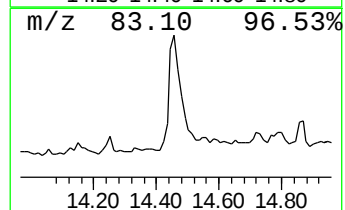
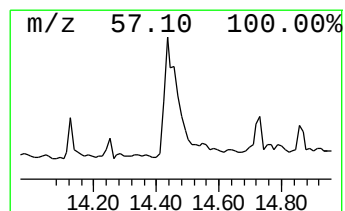
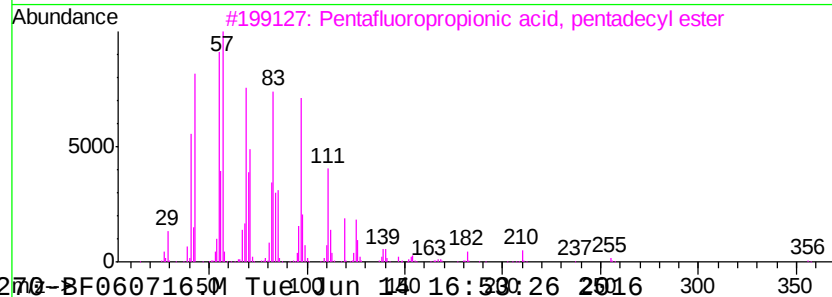
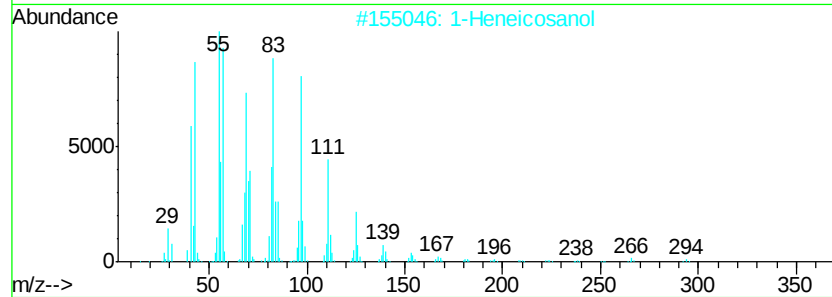
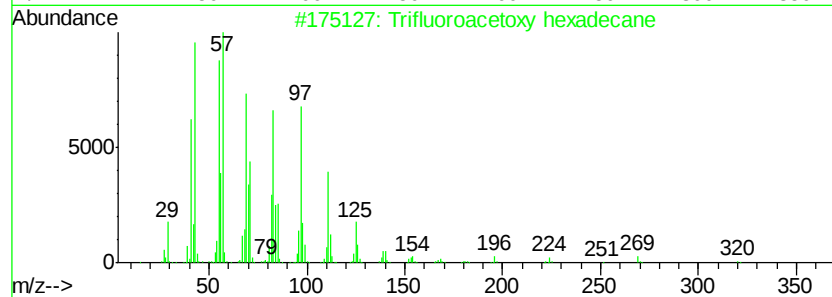
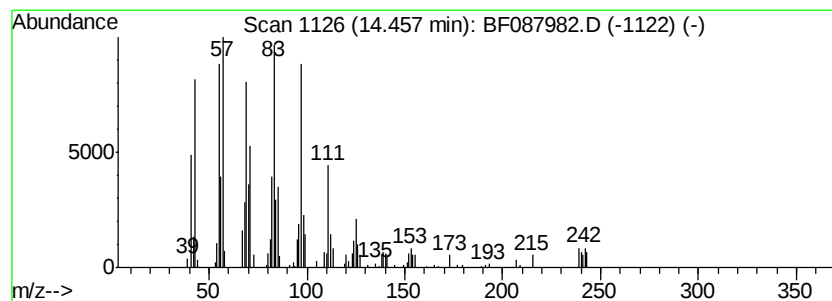
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ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.46	6.34 ng	230537	Chrysene-d12		13.94	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

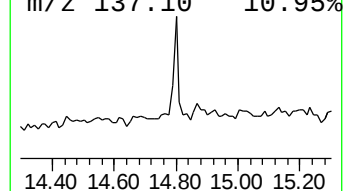
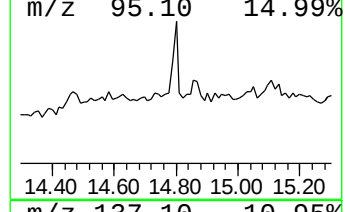
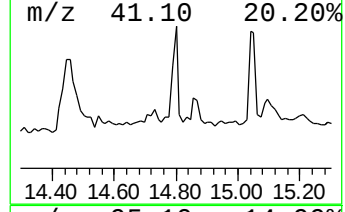
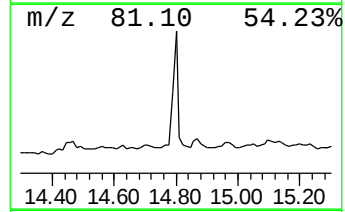
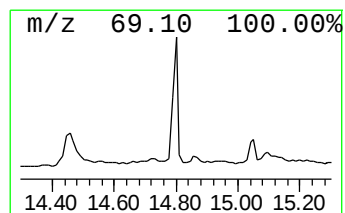
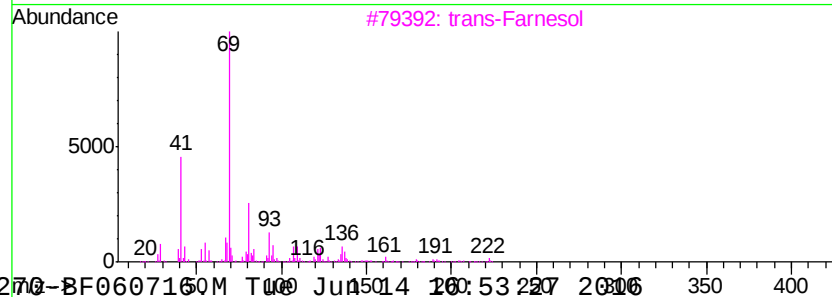
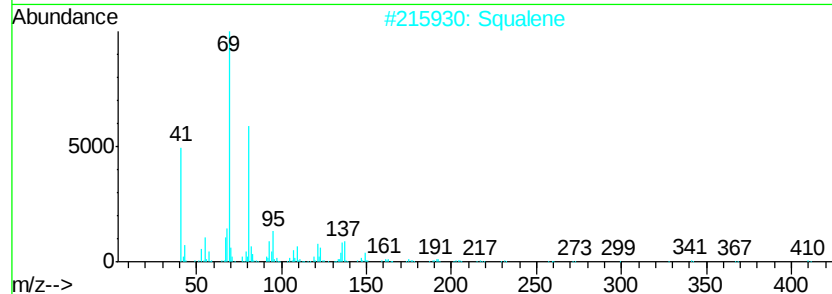
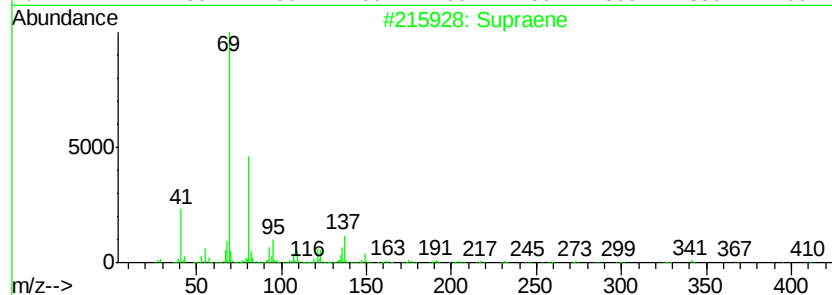
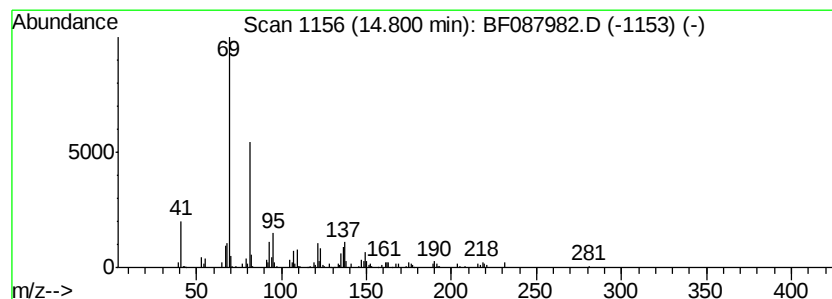
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ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Supraene Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.60 ng	84700	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Supraene		410 C30H50	007683-64-9 91
2	Squalene		410 C30H50	000111-02-4 91
3	trans-Farnesol		222 C15H26O	000106-28-5 78
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...		264 C17H28O2	004128-17-0 72
5	7,11-Dimethyldodeca-2,6,10-trien...		208 C14H24O	125529-10-4 72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
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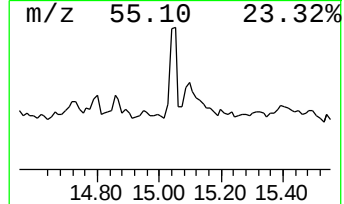
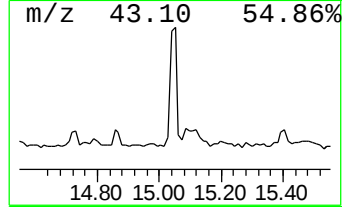
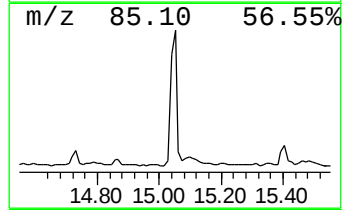
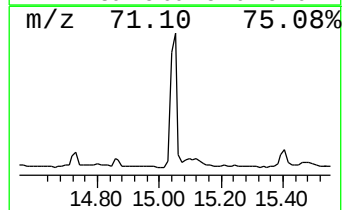
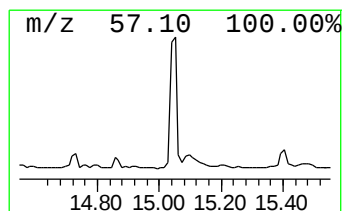
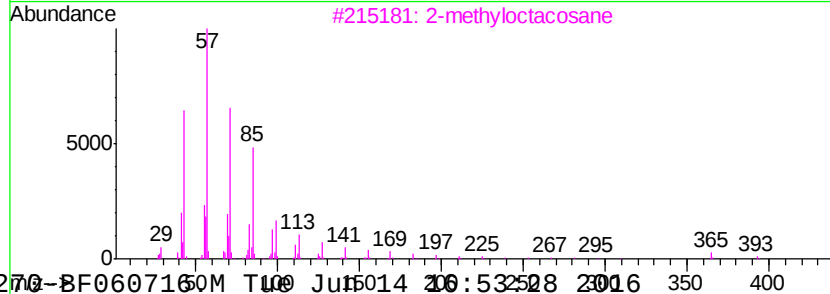
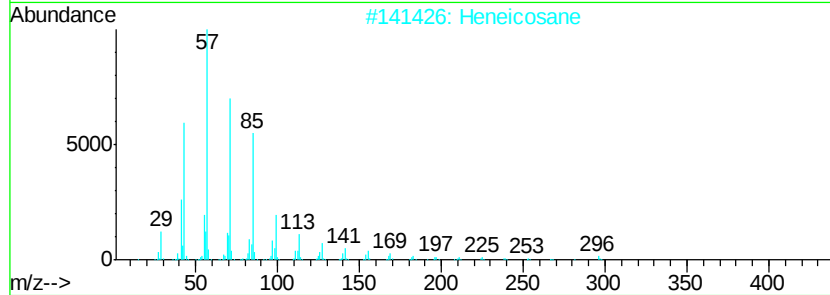
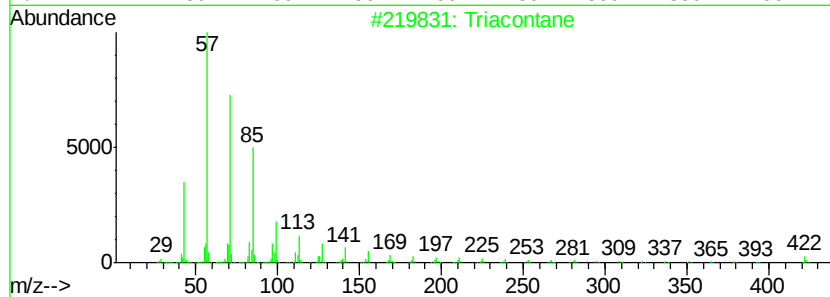
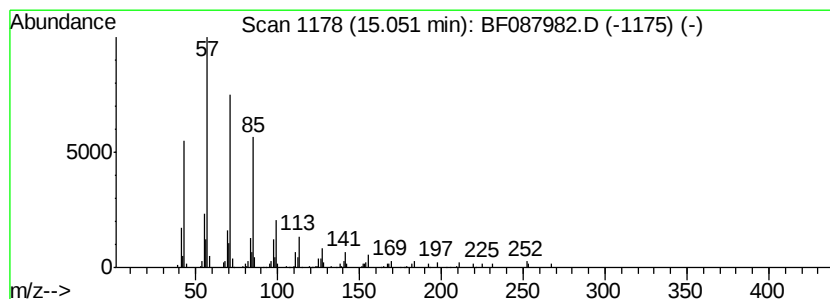
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ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Triacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.05	5.08 ng	165751	Perylene-d12		15.36
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

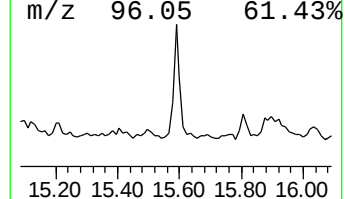
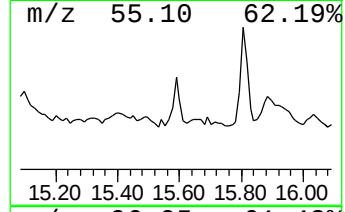
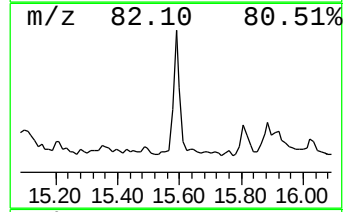
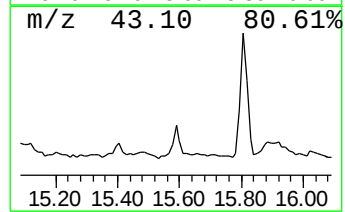
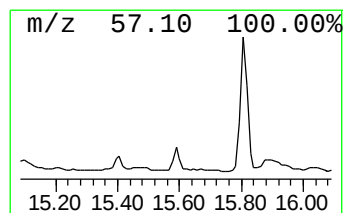
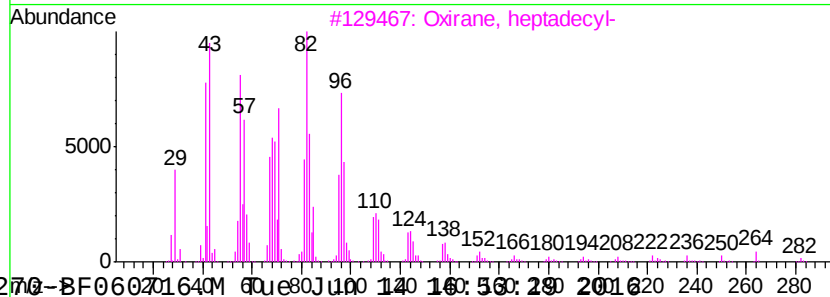
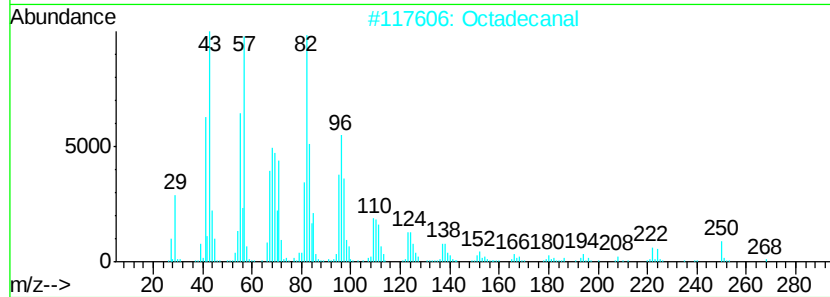
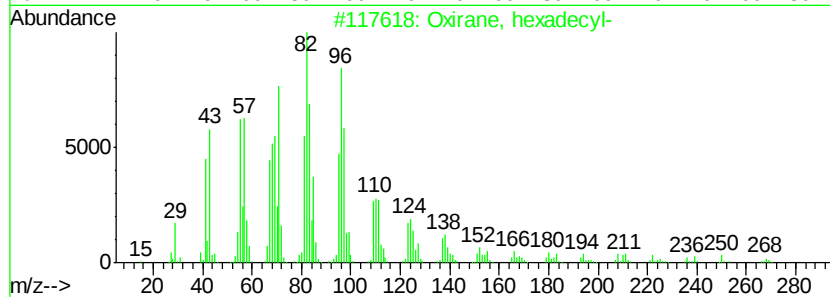
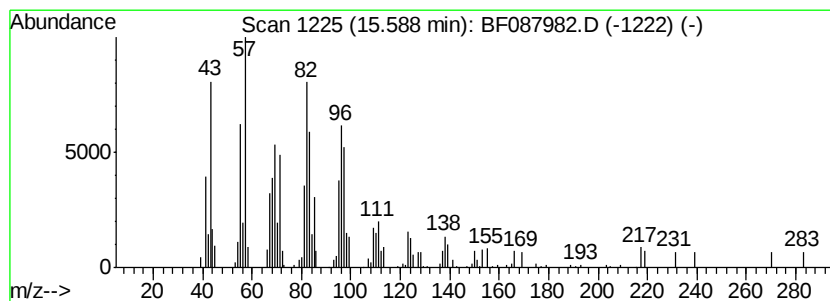
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ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Oxirane, hexadecyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.59	2.90 ng	94527	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2	Octadecanal	268	C18H36O	000638-66-4	83
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	83
4	Heptadecanal	254	C17H34O	1000376-70-0	64
5	Hexadecanal	240	C16H32O	000629-80-1	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
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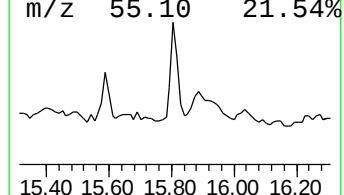
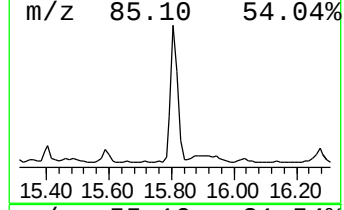
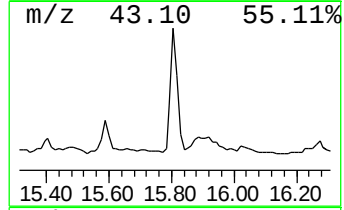
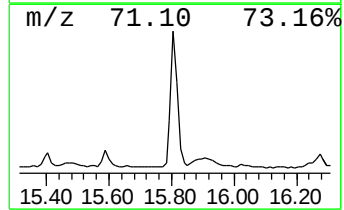
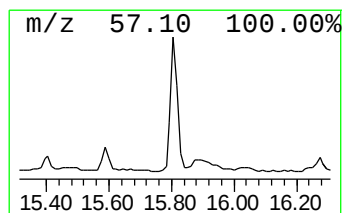
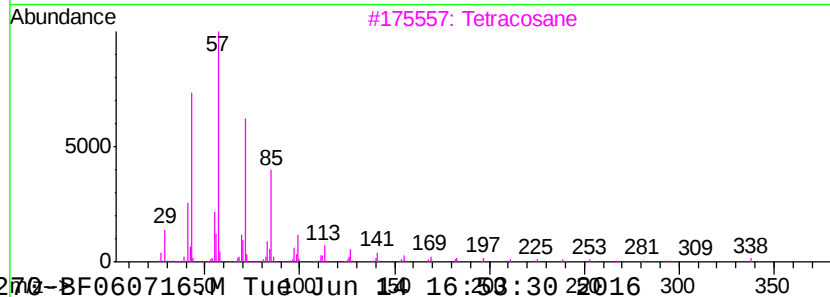
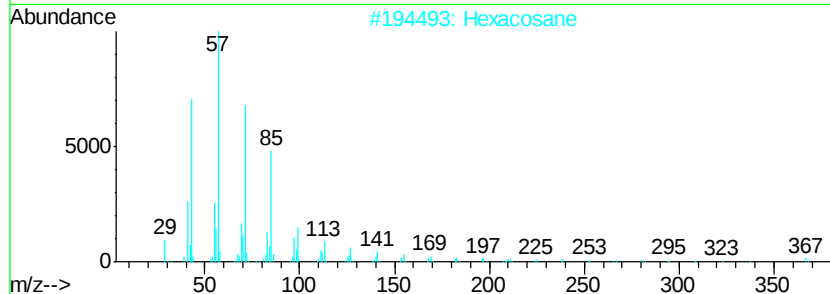
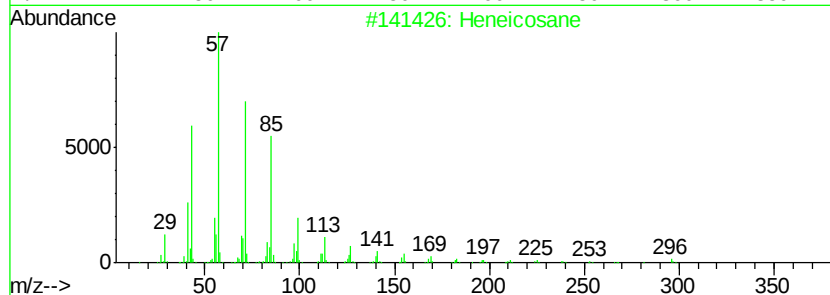
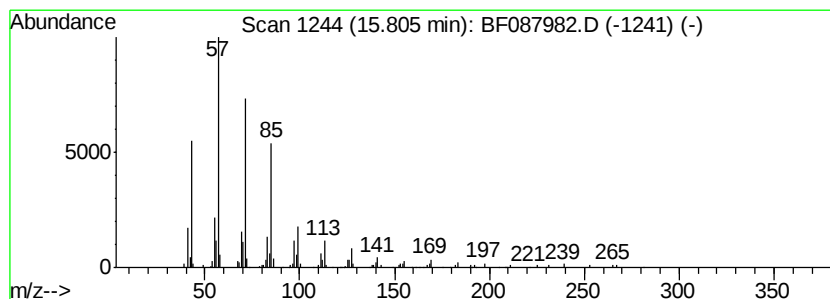
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ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.81	6.91 ng	225234	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Docosane	310	C22H46	000629-97-0	91
5	Heptadecane	240	C17H36	000629-78-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
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Sample : H3449-07
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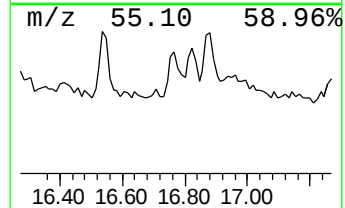
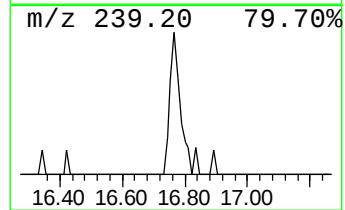
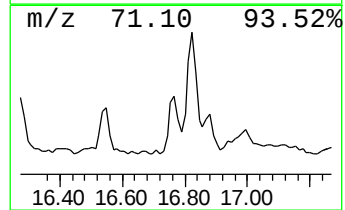
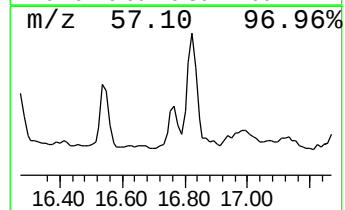
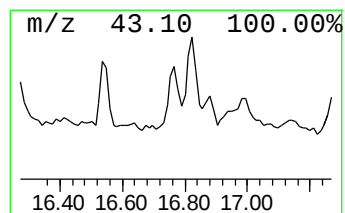
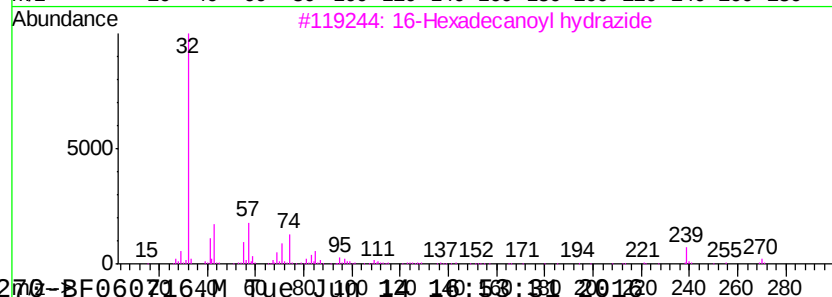
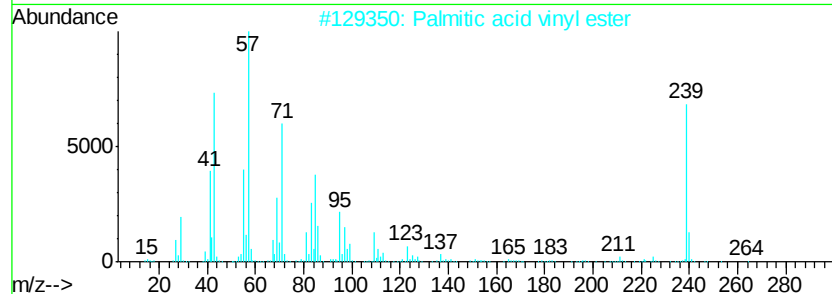
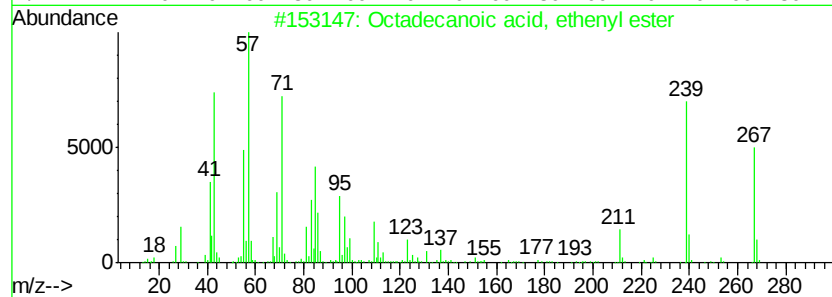
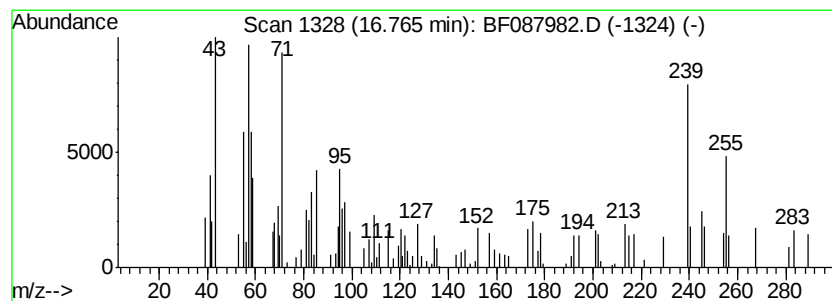
Instrument :
BNA_F
ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown16.77 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.77	2.25 ng	73478	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	47
2	Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	35
3	16-Hexadecanoyl hydrazide	270	C16H34N2O	002619-88-7	35
4	Stearic acid hydrazide	298	C18H38N2O	004130-54-5	14
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

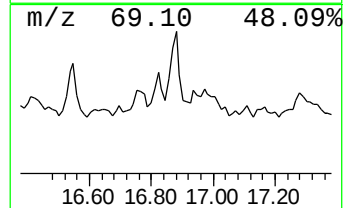
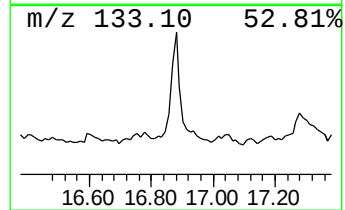
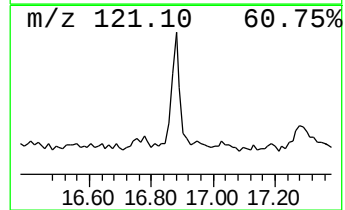
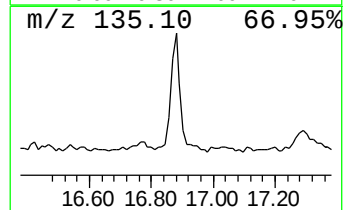
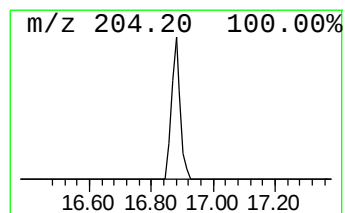
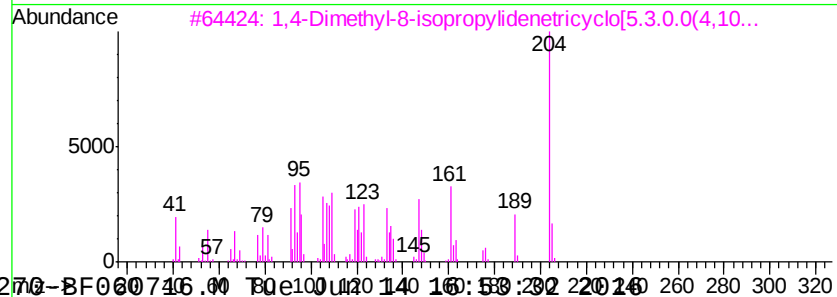
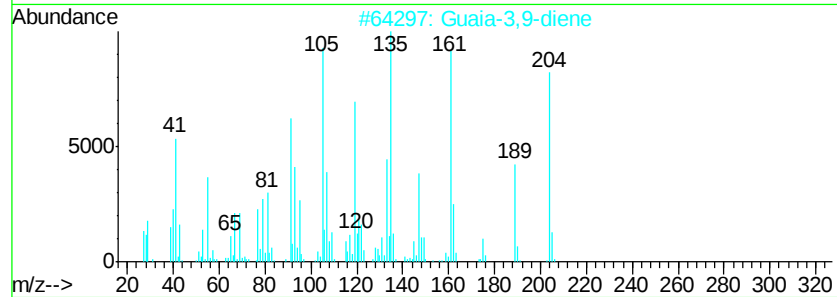
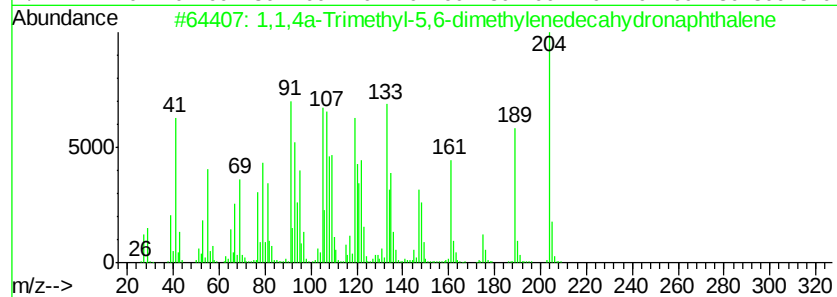
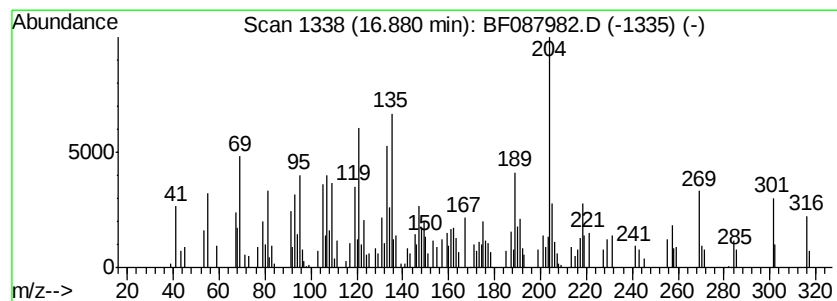
Instrument :
BNA_F
ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.88	5.08 ng	165824	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	70
2	Guaia-3,9-diene	204	C15H24	000489-83-8	53
3	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	50
4	1,2,4,8-Tetramethylbicyclo[6.3.0]...	204	C15H24	137235-51-9	49
5	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
 Data File : BF087982.D
 Acq On : 13 Jun 2016 14:37
 Operator : UM/SJ
 Sample : H3449-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

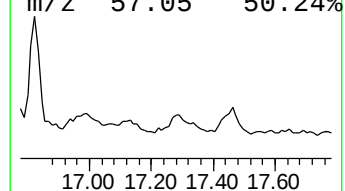
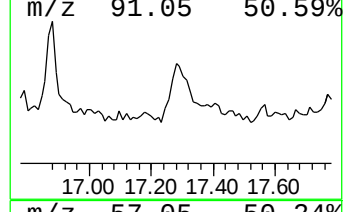
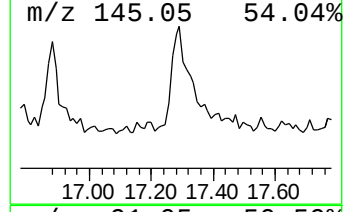
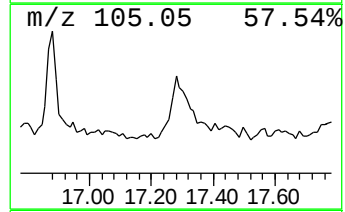
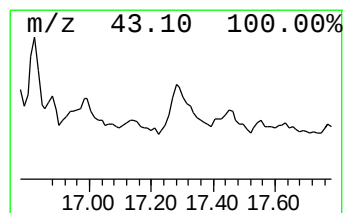
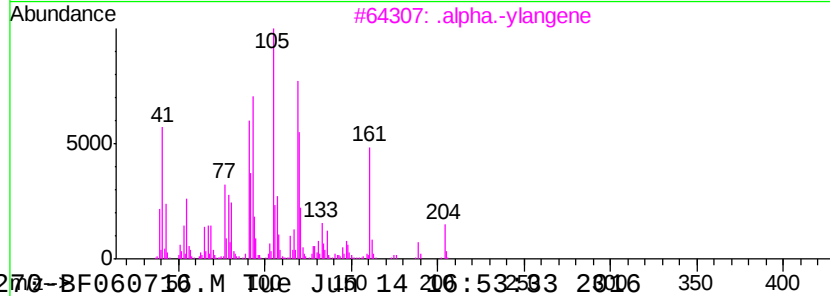
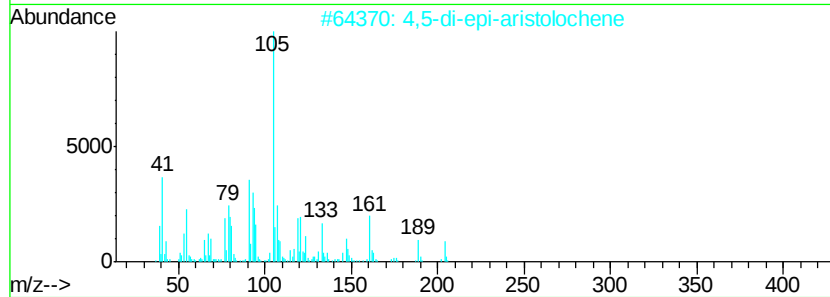
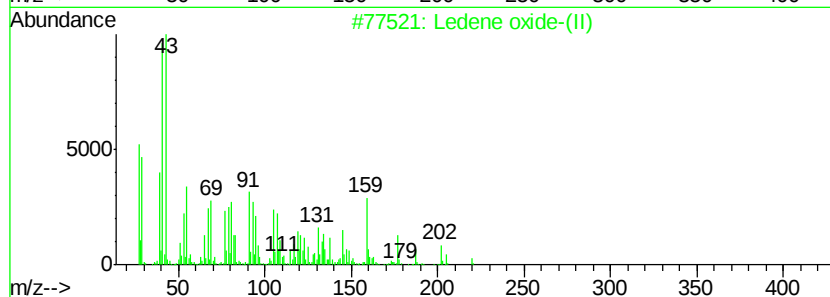
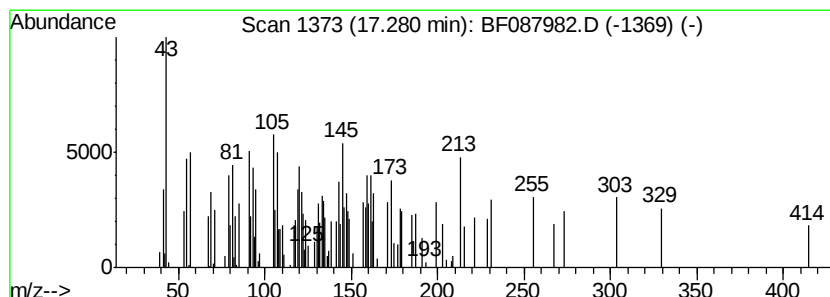
Instrument :
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 ClientSampleId :
 19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 17 unknown17.28 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	4.82 ng	157154	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Ledene oxide-(II)	220 C15H24O	1000159-36-7 14
2		4,5-di-epi-aristolochene	204 C15H24	1000374-17-1 11
3		.alpha.-ylangene	204 C15H24	1000374-19-0 10
4		Strophanthidol, 3,19-diacetate	490 C27H38O8	083349-11-5 10
5		1H-Pyrrole-1-carboxylic acid, 2-...	329 C15H24BrN02	168106-33-0 10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

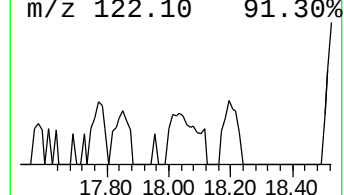
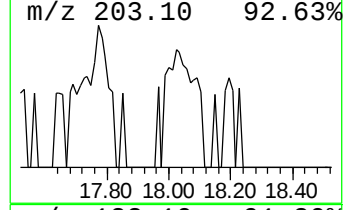
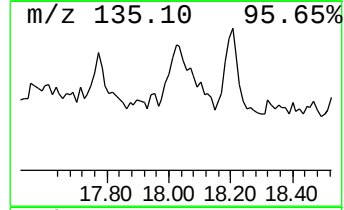
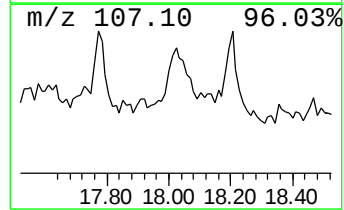
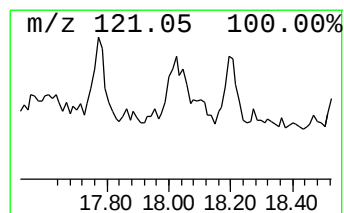
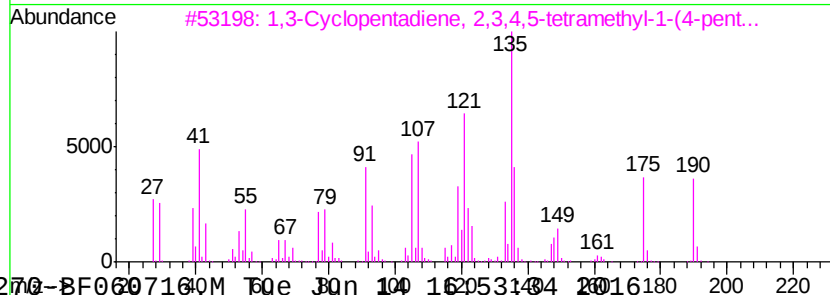
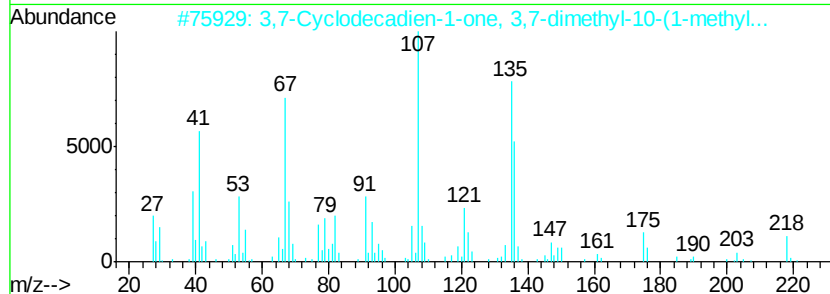
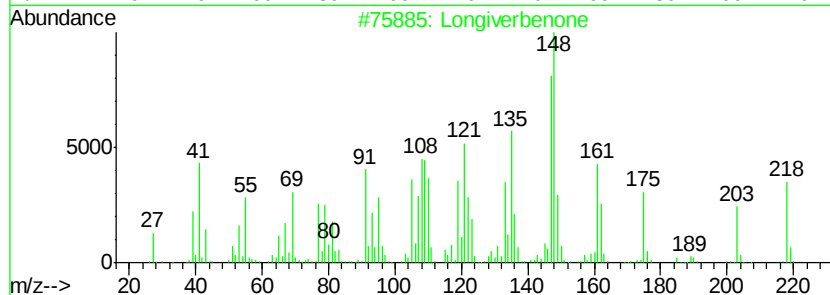
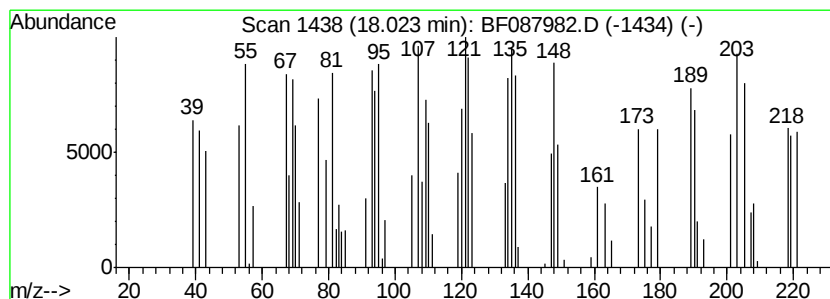
Instrument :
BNA_F
ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown18.02 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.02	2.74 ng	89320	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Longiverbenone	218	C15H22O	064180-68-3	45
2	3,7-Cyclodecadien-1-one, 3,7-dim...	218	C15H22O	006902-91-6	18
3	1,3-Cyclopentadiene, 2,3,4,5-tet...	190	C14H22	1000161-28-7	18
4	Pvrazine, 2,5-diethyl-	136	C8H12N2	013238-84-1	18
5	cis-2-(2-Pentenyl)furan	136	C9H12O	070424-13-4	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

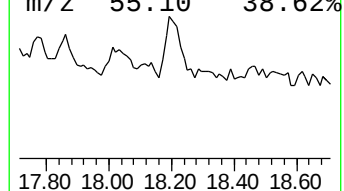
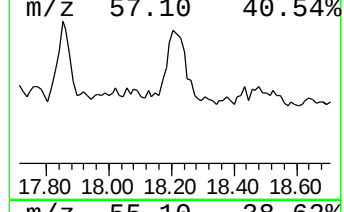
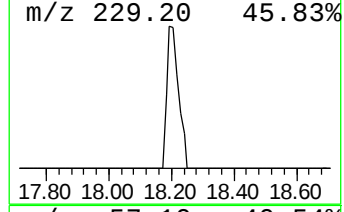
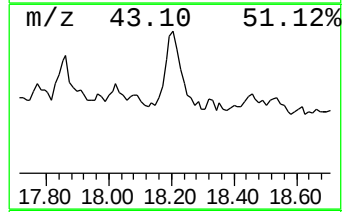
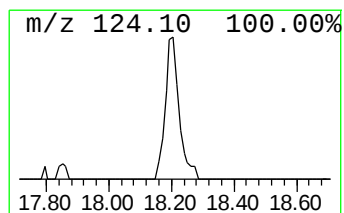
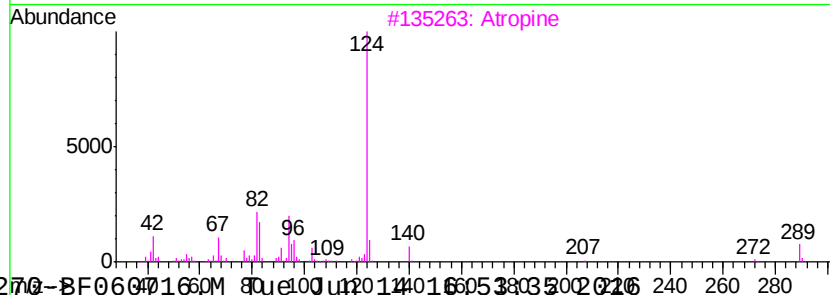
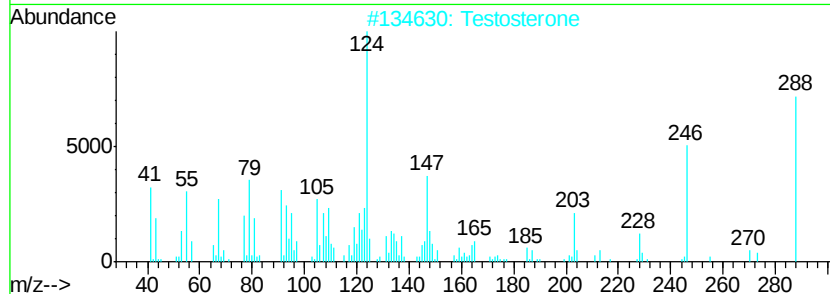
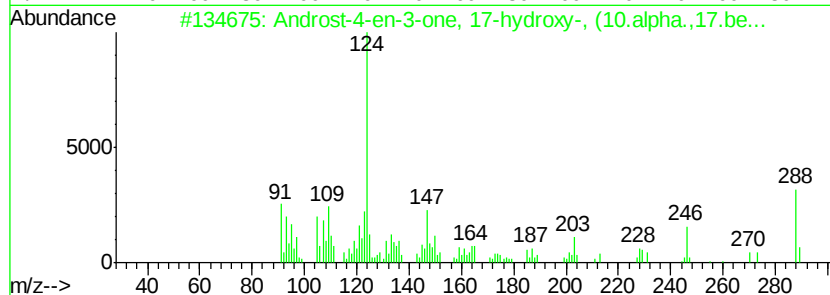
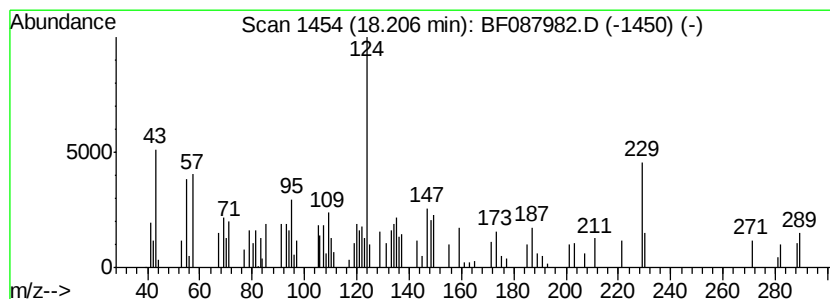
Instrument :
BNA_F
ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 unknown18.21 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.21	3.98 ng	129670	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Androst-4-en-3-one, 17-hydroxy-, ...	288	C19H28O2	000604-39-7	46
2	Testosterone	288	C19H28O2	000058-22-0	46
3	Atropine	289	C17H23NO3	000051-55-8	22
4	Pvrazine, 2-methoxy-3-(2-methylvp...	166	C9H14N2O	024683-00-9	22
5	Thiophene-2-sulfonic acid, (3-fl...	271	C11H10FN02S2	1000311-21-1	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
19-VE-PILE-WALL(0-2)

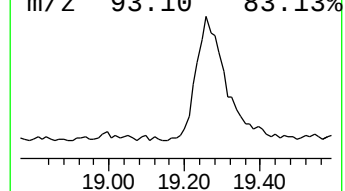
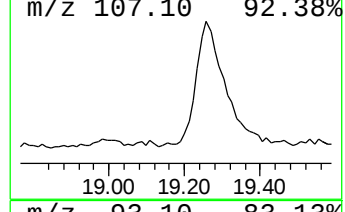
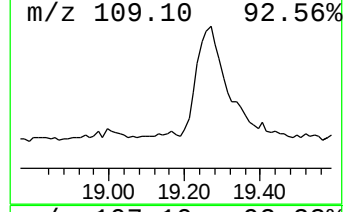
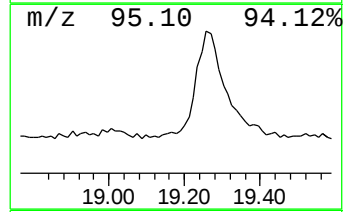
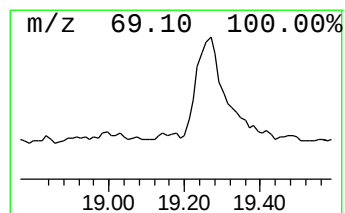
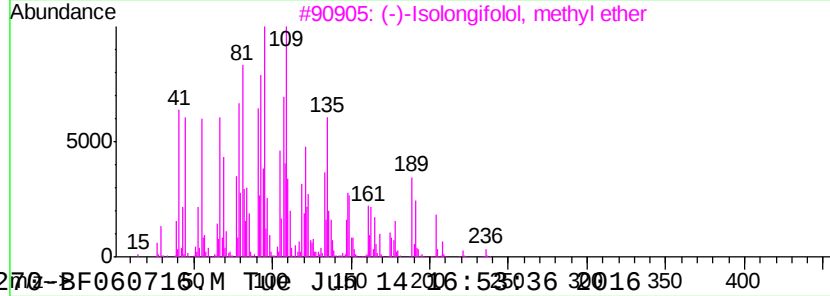
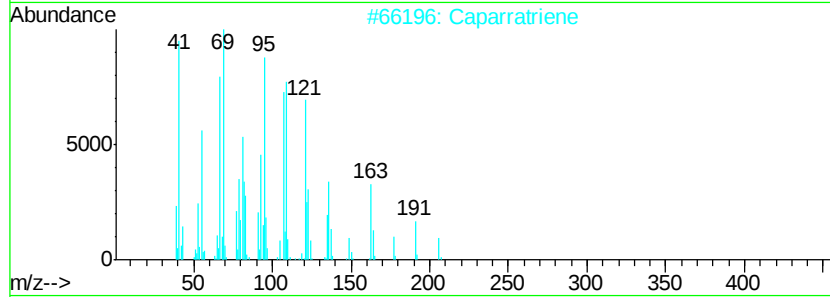
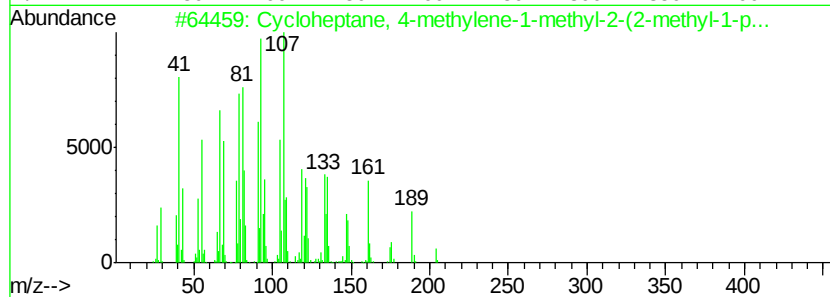
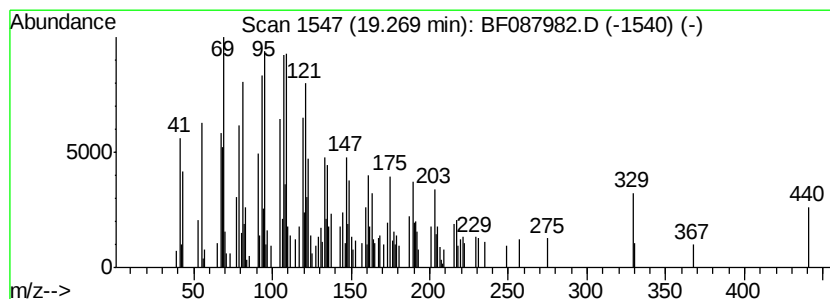
Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Cycloheptane, 4-methylene-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	15.55 ng	507172	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	86
2		Caparratriene	206	C15H26	1000374-08-7	83
3		(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	38
4		1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	38
5		4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061316\
Data File : BF087982.D
Acq On : 13 Jun 2016 14:37
Operator : UM/SJ
Sample : H3449-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
19-VE-PILE-WALL(0-2)

Quant Title :

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.02	5.9	ng	197209	1	6.79	671583	20.0
2-Pentanone, 4-hy...	4.97	7.2	ng	240664	1	6.79	671583	20.0
unknown6.56	6.56	69.9	ng	2346800	1	6.79	671583	20.0
n-Hexadecanoic acid	11.85	5.5	ng	257567	4	11.31	940836	20.0
Hexadecanoic acid...	12.73	3.2	ng	115727	5	13.94	727365	20.0
1-Heneicosanol	13.82	7.5	ng	273559	5	13.94	727365	20.0
Trifluoroacetoxy ...	14.46	6.3	ng	230537	5	13.94	727365	20.0
Supraene	14.80	2.6	ng	84700	6	15.36	652377	20.0
triacontane	15.05	5.1	ng	165751	6	15.36	652377	20.0
Oxirane, hexadecyl-	15.59	2.9	ng	94527	6	15.36	652377	20.0
Heneicosane	15.81	6.9	ng	225234	6	15.36	652377	20.0
unknown16.77	16.77	2.3	ng	73478	6	15.36	652377	20.0
1,1,4a-Trimethyl-...	16.88	5.1	ng	165824	6	15.36	652377	20.0
unknown17.28	17.28	4.8	ng	157154	6	15.36	652377	20.0
unknown18.02	18.02	2.7	ng	89320	6	15.36	652377	20.0
unknown18.21	18.21	4.0	ng	129670	6	15.36	652377	20.0
Cycloheptane, 4-m...	19.27	15.6	ng	507172	6	15.36	652377	20.0