

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
 Data File : BF110229.D
 Acq On : 27 Oct 2018 00:06
 Operator : JU/SJ
 Sample : J5639-13
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BS-DRUM

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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	2.316	33	39	47	rVB	1619672	2137794	69.06%	8.440%
2	5.198	526	529	539	rVB	46712	57065	1.84%	0.225%
3	5.587	591	595	606	rBV	1478292	1411938	45.61%	5.574%
4	6.587	761	765	776	rBV2	994480	1044624	33.75%	4.124%
5	6.740	786	791	794	rBV	2628545	2499129	80.73%	9.866%
6	6.798	798	801	805	rVB	46152	46699	1.51%	0.184%
7	6.969	826	830	833	rBV	922384	785599	25.38%	3.101%
8	7.128	852	857	860	rBV	2504854	2382090	76.95%	9.404%
9	7.228	870	874	882	rVB	57940	50462	1.63%	0.199%
10	7.534	920	926	929	rBV	1905224	1854880	59.92%	7.323%
11	7.757	956	964	969	rBV	144180	220321	7.12%	0.870%
12	8.251	1044	1048	1053	rBV	1106646	929733	30.04%	3.670%
13	8.522	1089	1094	1101	rBV3	23921	40285	1.30%	0.159%
14	8.869	1150	1153	1159	rBV	179419	143110	4.62%	0.565%
15	8.969	1166	1170	1172	rVB2	24133	32490	1.05%	0.128%
16	9.328	1224	1231	1234	rBV	3375380	3095478	100.00%	12.220%
17	9.716	1294	1297	1300	rBV	47487	38791	1.25%	0.153%
18	10.010	1342	1347	1355	rVB2	1049011	920925	29.75%	3.636%
19	10.181	1368	1376	1380	rBV	26103	33767	1.09%	0.133%
20	10.381	1407	1410	1415	rBV3	64205	72884	2.35%	0.288%
21	10.669	1454	1459	1463	rBV	88949	71874	2.32%	0.284%
22	10.804	1478	1482	1490	rBV	1526011	1390653	44.93%	5.490%
23	11.504	1597	1601	1609	rBV	890471	750853	24.26%	2.964%
24	11.633	1620	1623	1634	rBV	1247607	1143053	36.93%	4.513%
25	12.010	1683	1687	1692	rBV2	22803	32901	1.06%	0.130%
26	13.092	1866	1871	1874	rBV	2465318	2337086	75.50%	9.226%
27	13.851	1997	2000	2004	rBV	445418	359172	11.60%	1.418%
28	13.969	2017	2020	2025	rBV	63345	74836	2.42%	0.295%
29	14.151	2047	2051	2057	rBV	682050	620523	20.05%	2.450%
30	14.592	2123	2126	2133	rVB2	44540	51608	1.67%	0.204%
31	14.916	2178	2181	2184	rVB	62552	60450	1.95%	0.239%
32	15.268	2237	2241	2247	rVB	66680	81393	2.63%	0.321%
33	15.680	2306	2311	2316	rVB	340009	480095	15.51%	1.895%
34	16.133	2385	2388	2394	rVB3	50615	78206	2.53%	0.309%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

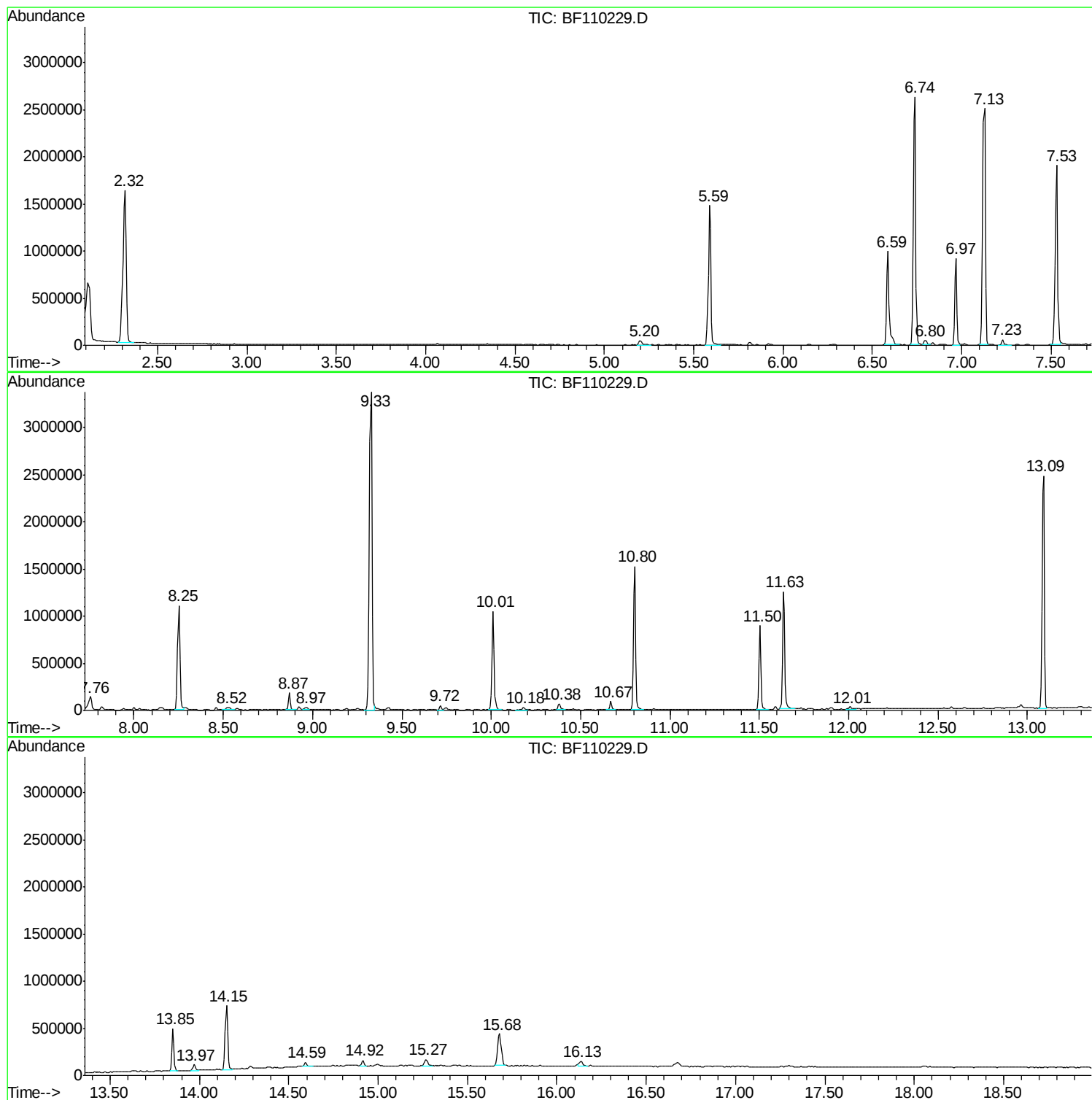
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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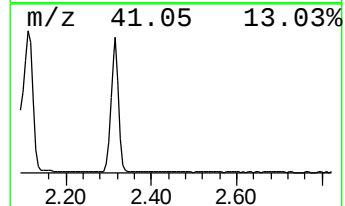
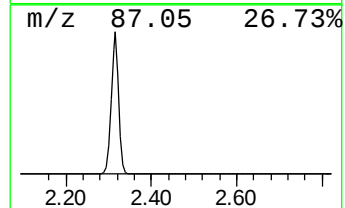
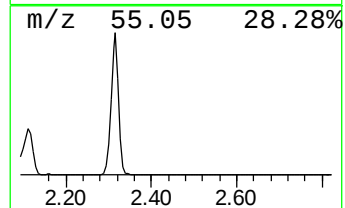
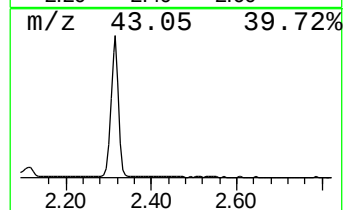
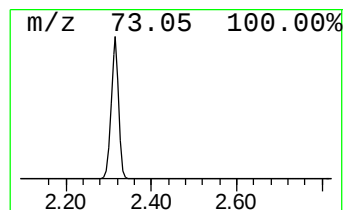
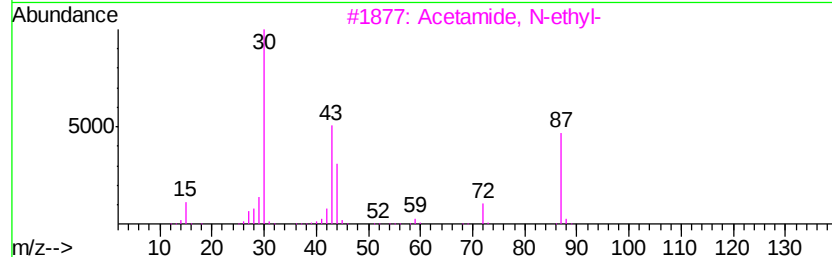
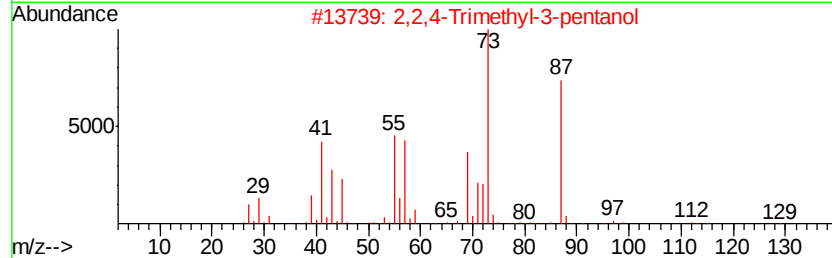
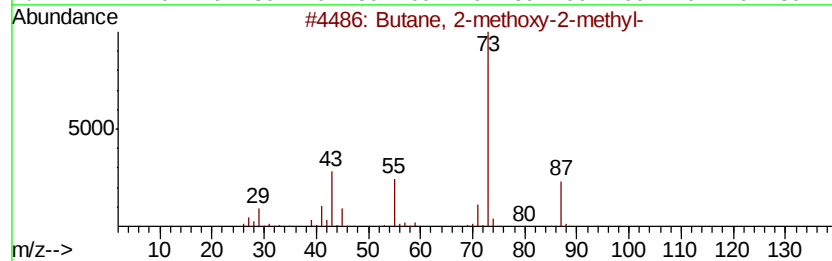
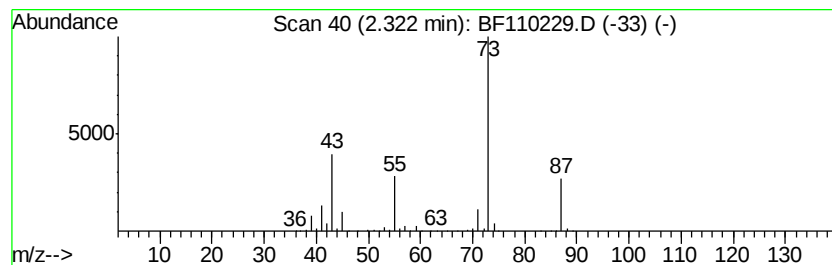
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	54.42 ng	2137790	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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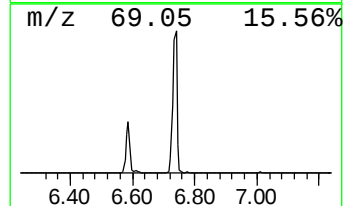
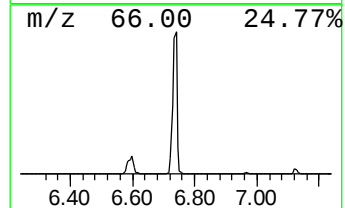
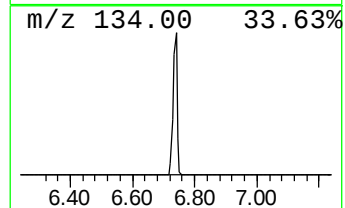
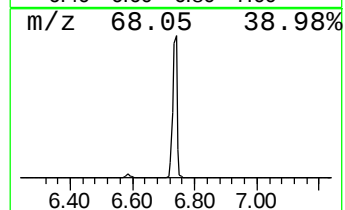
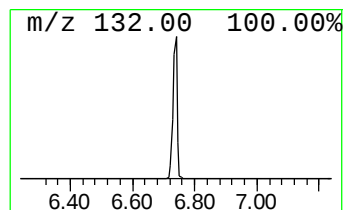
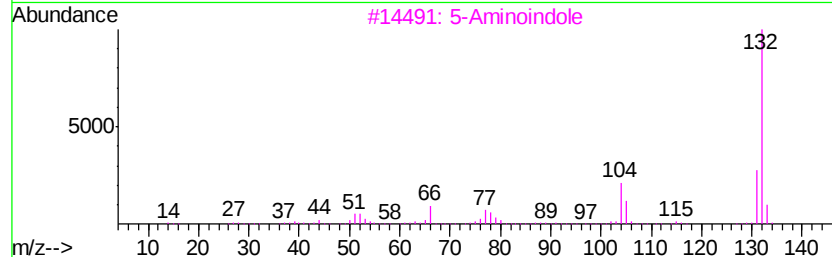
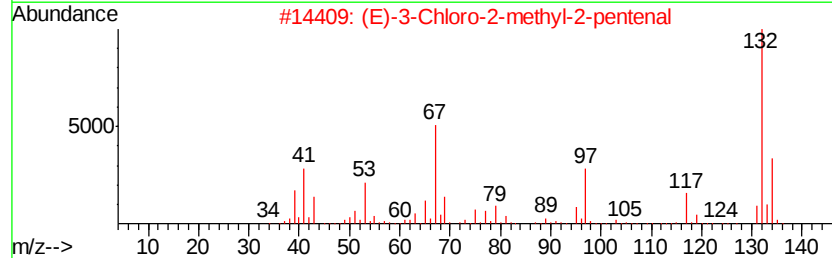
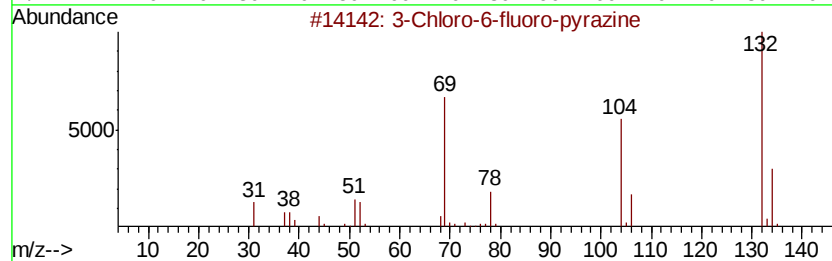
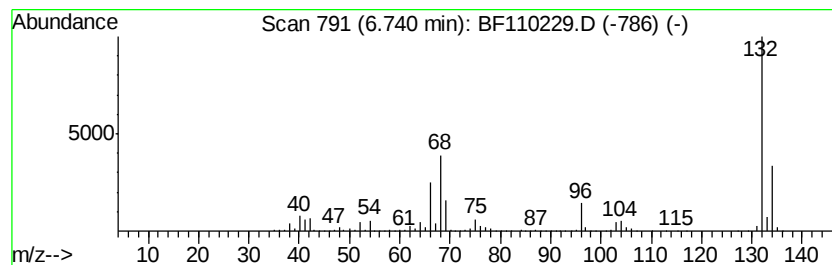
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	63.62 ng	2499130	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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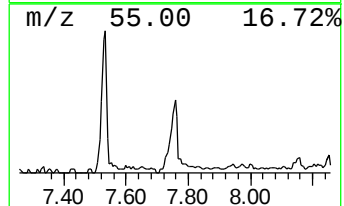
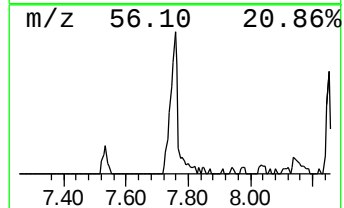
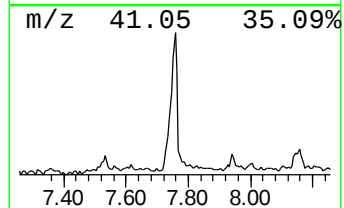
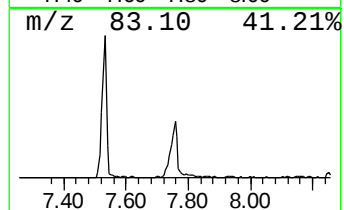
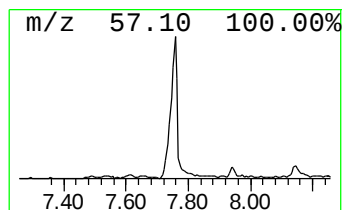
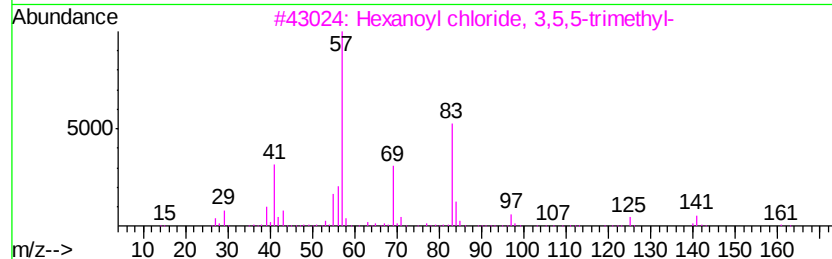
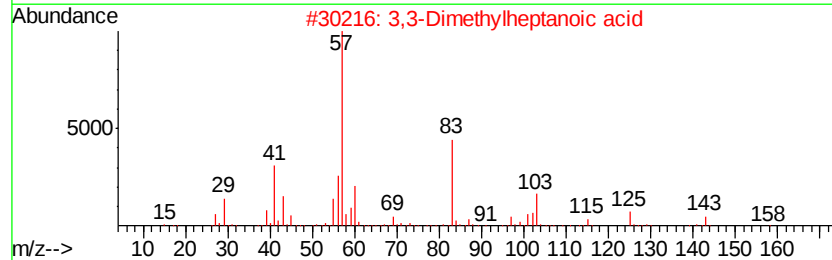
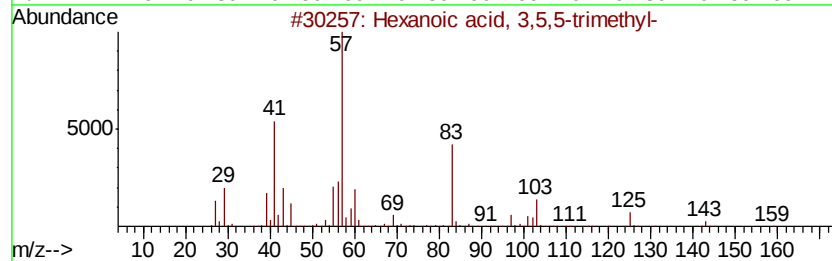
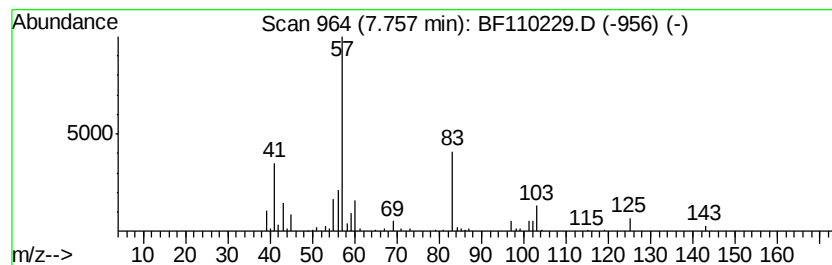
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Hexanoic acid, 3,5,5-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.76	4.74 ng	220321	Naphthalene-d8	8.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2			3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3			Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	42
4			Propanoic acid, 2,2-dimethyl-, h...	200	C12H24O2	017660-61-6	35
5			Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	32



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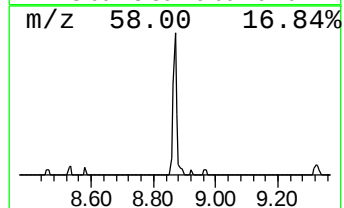
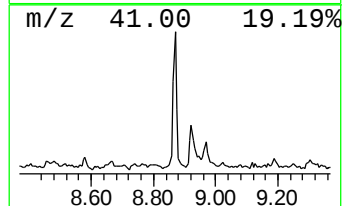
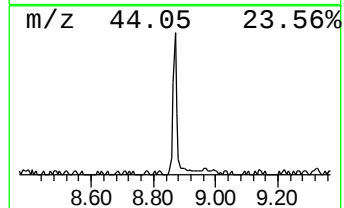
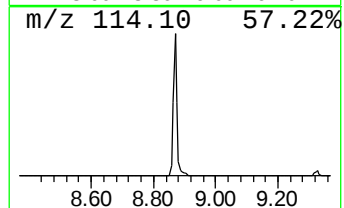
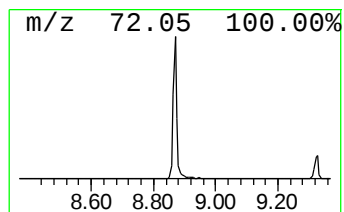
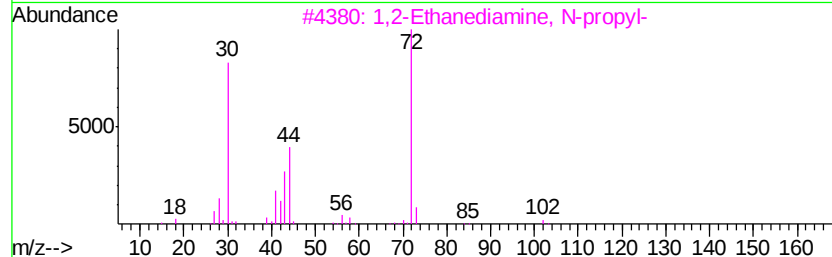
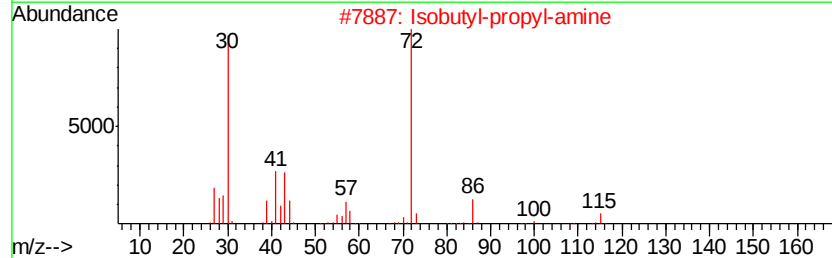
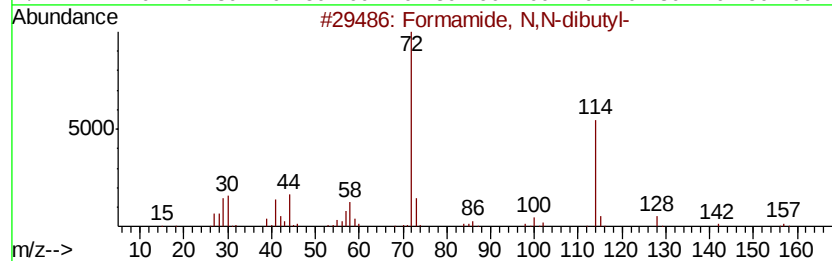
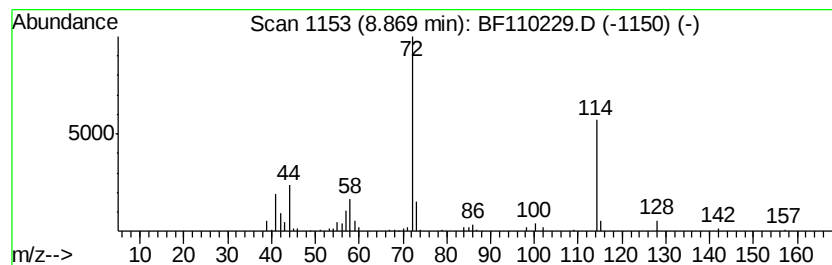
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Formamide, N,N-dibutyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.87	3.08 ng	143110	Naphthalene-d8	8.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Formamide, N,N-dibutyl-	157	C9H19NO	000761-65-9	87
2		Isobutyl-propyl-amine	115	C7H17N	039190-66-4	47
3		1,2-Ethanediamine, N-propyl-	102	C5H14N2	000111-39-7	46
4		Diisopropylethylamine	129	C8H19N	007087-68-5	43
5		Dimethyl(2-octyl)amine	157	C10H23N	007378-97-4	43



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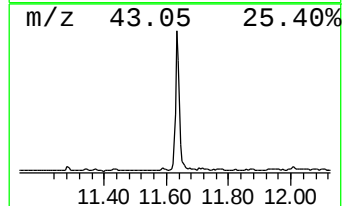
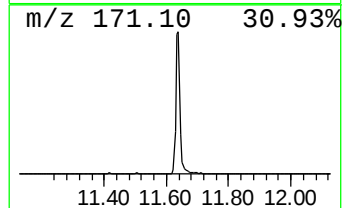
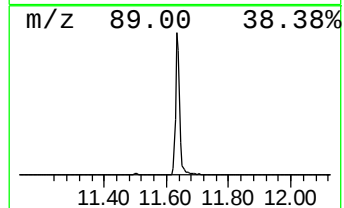
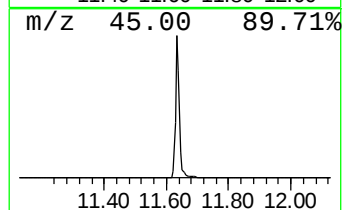
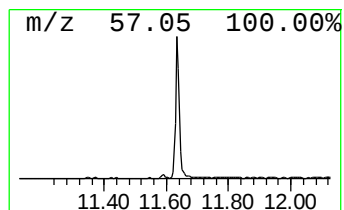
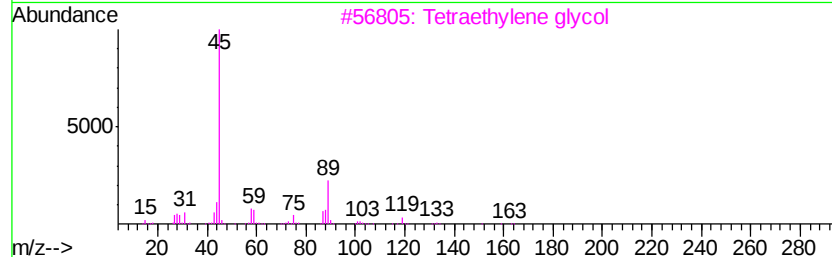
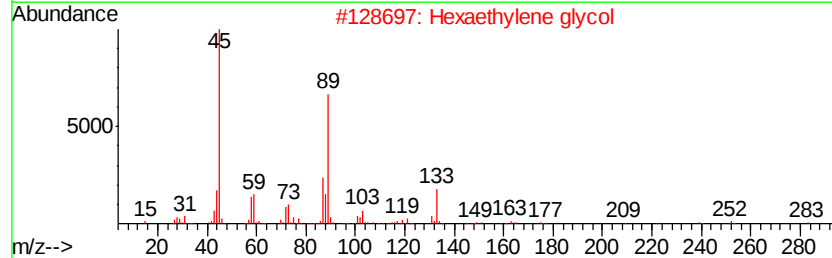
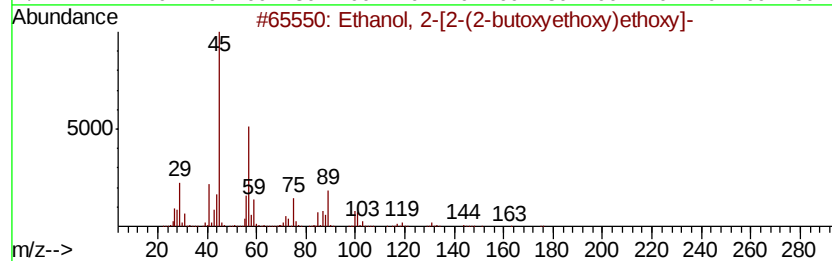
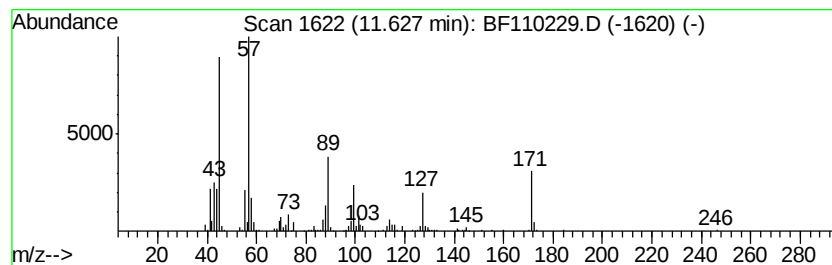
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Peak Number 6 unknown11.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	30.45 ng	1143050	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	47
2		Hexaethylene glycol	282	C12H26O7	002615-15-8	43
3		Tetraethylene glycol	194	C8H18O5	000112-60-7	38
4		1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	38
5		Pentaethylene glycol	238	C10H22O6	004792-15-8	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110229.D
Acq On : 27 Oct 2018 00:06
Operator : JU/SJ
Sample : J5639-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BS-DRUM

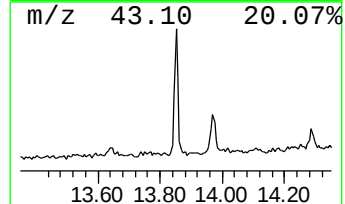
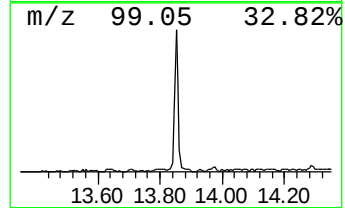
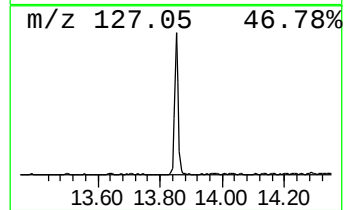
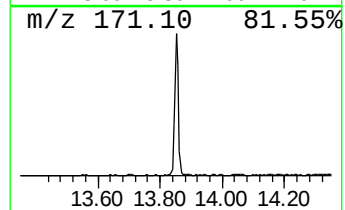
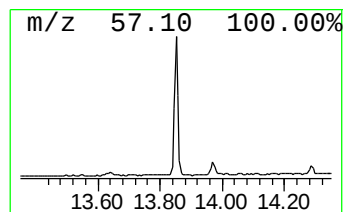
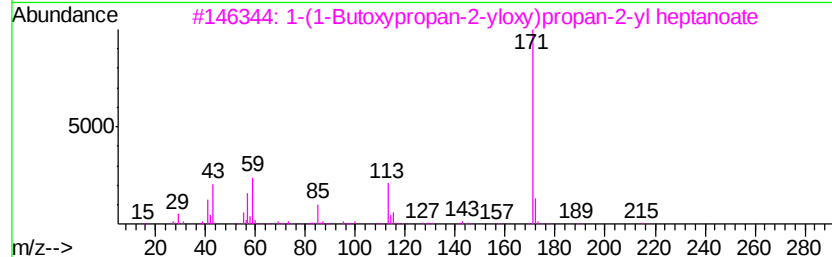
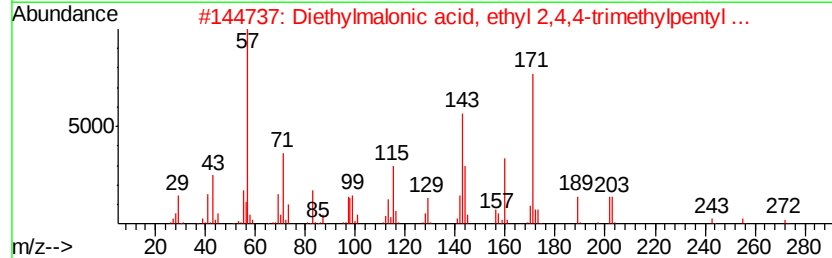
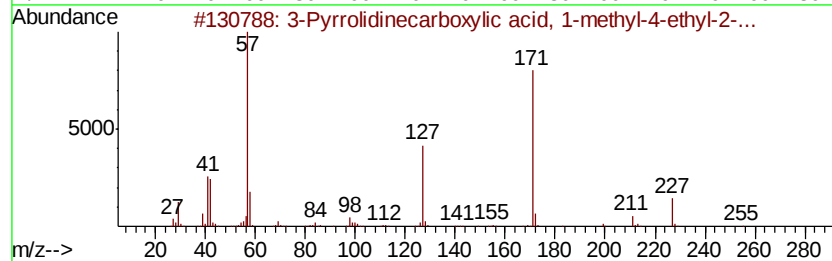
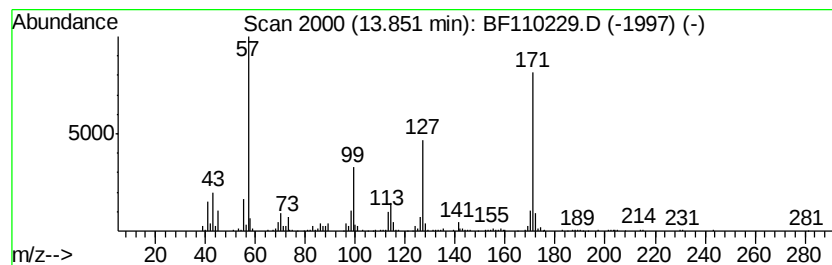
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Pyrrolidinecarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	11.58 ng	359172	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pyrrolidinecarboxylic acid, 1-...	284	C15H28N2O3	1000196-95-3	53
2		Diethylmalonic acid, ethyl 2,4,4...	300	C17H32O4	1000369-47-3	42
3		1-(1-Butoxypropan-2-yloxy)propan...	302	C17H34O4	1000367-12-8	38
4		2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	35
5		2,6-Difluorophenyl isocyanate	171	C7H3F2NS	065295-69-4	35



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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BS-DRUM

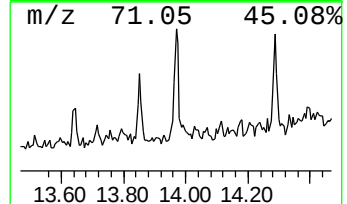
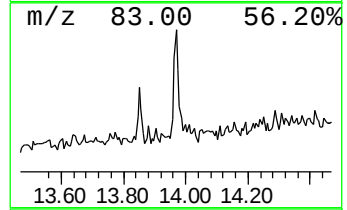
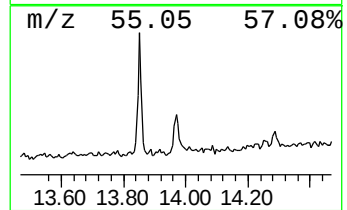
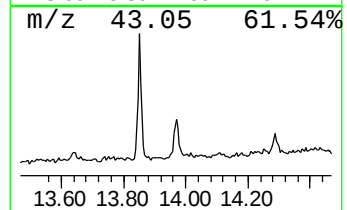
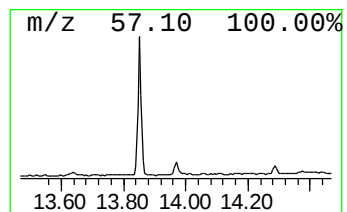
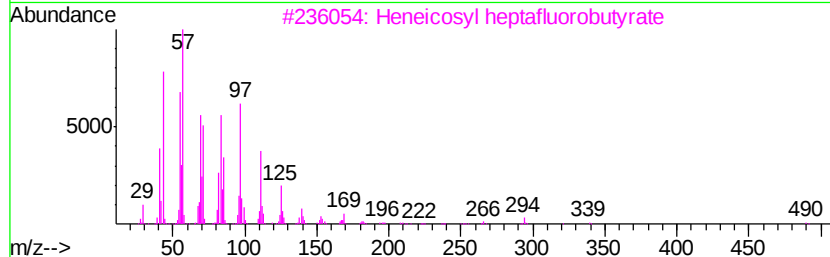
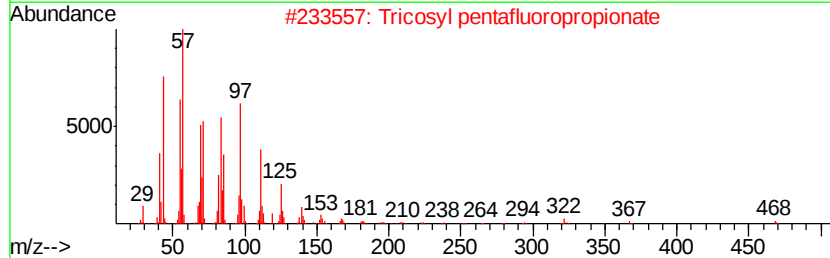
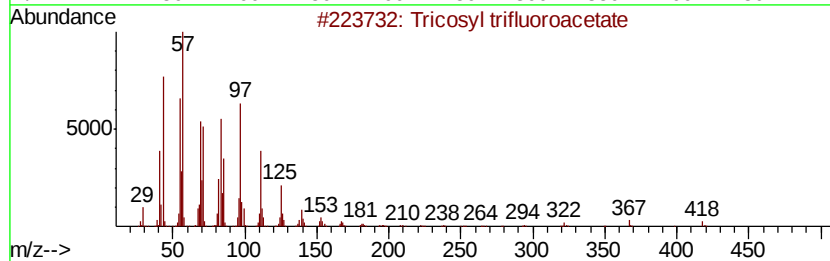
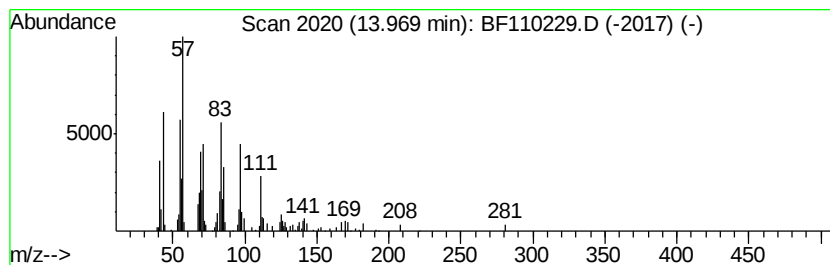
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tricosyl trifluoroacetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.41 ng	74836	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	94
2		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
3		Heneicosyl heptafluorobutvrate	508	C25H43F7O2	1000351-83-8	91
4		Tricosyl heptafluorobutvrate	536	C27H47F7O2	1000351-83-4	91
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
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Sample : J5639-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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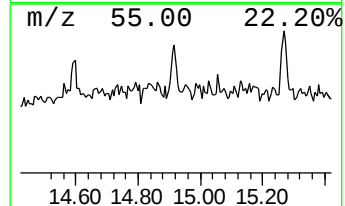
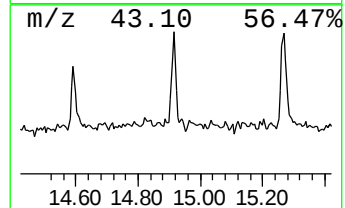
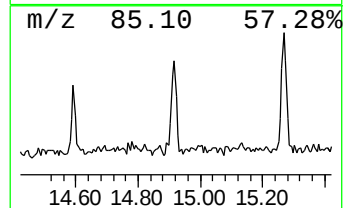
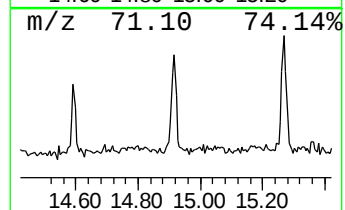
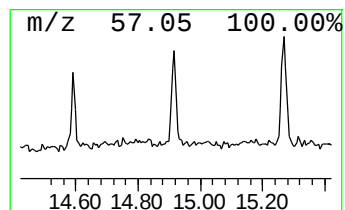
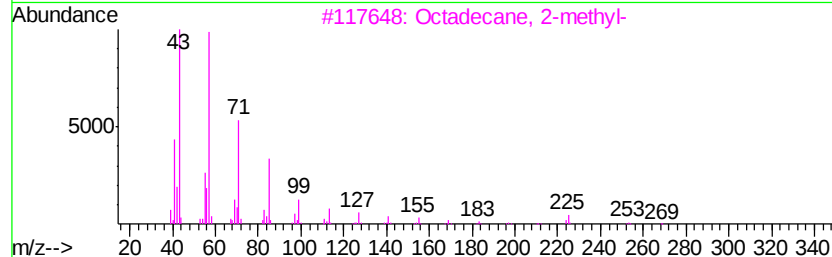
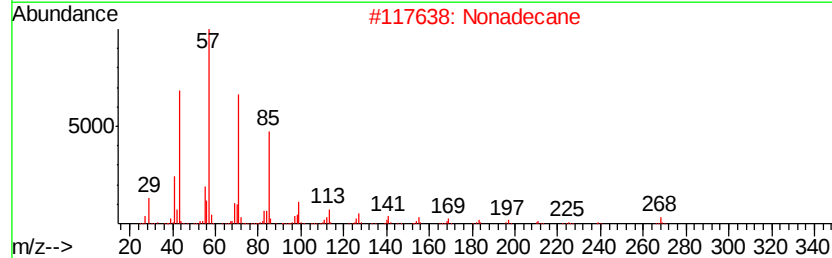
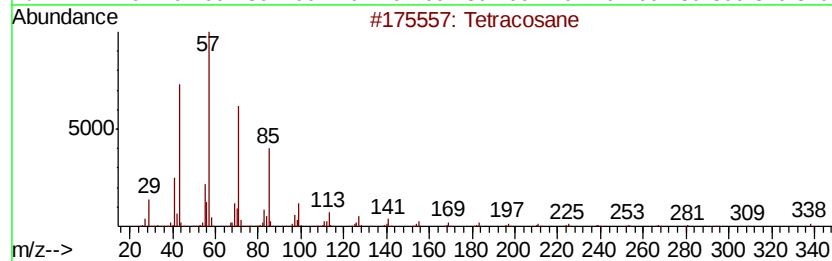
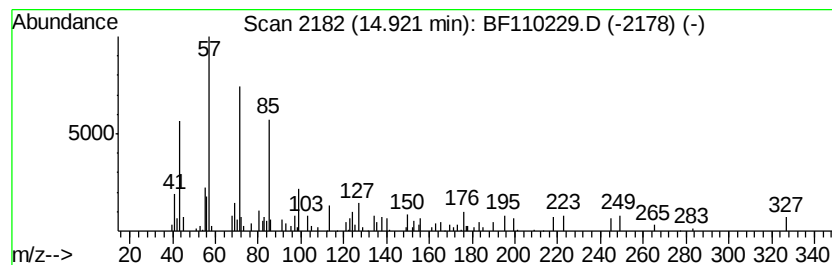
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.52 ng	60450	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	87
2		Nonadecane	268	C19H40	000629-92-5	80
3		Octadecane, 2-methyl-	268	C19H40	001560-88-9	78
4		Heneicosane	296	C21H44	000629-94-7	74
5		Pentadecane	212	C15H32	000629-62-9	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110229.D
Acq On : 27 Oct 2018 00:06
Operator : JU/SJ
Sample : J5639-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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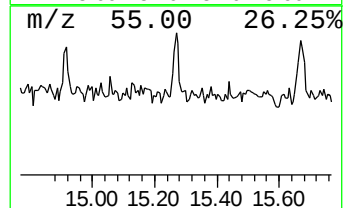
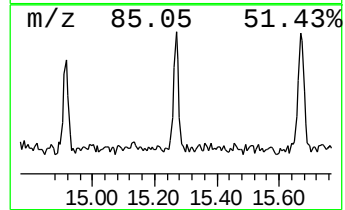
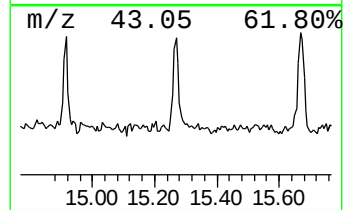
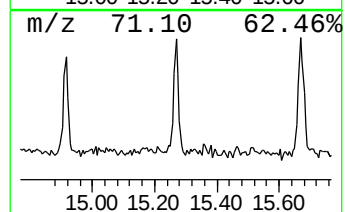
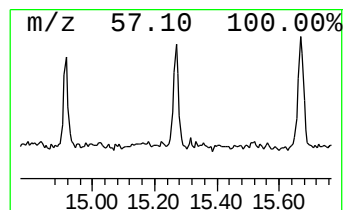
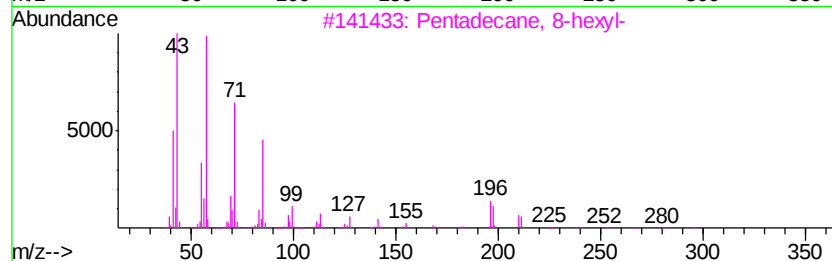
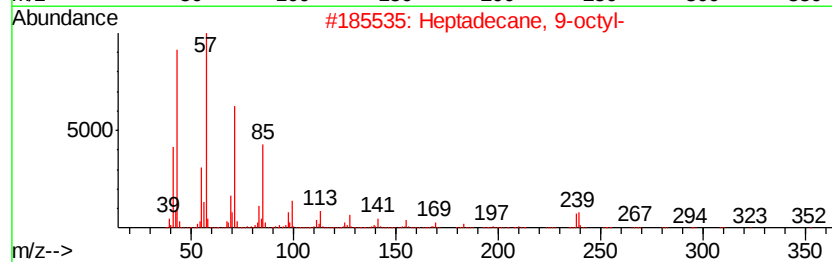
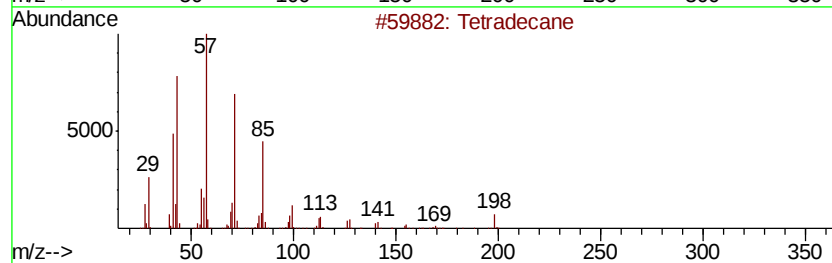
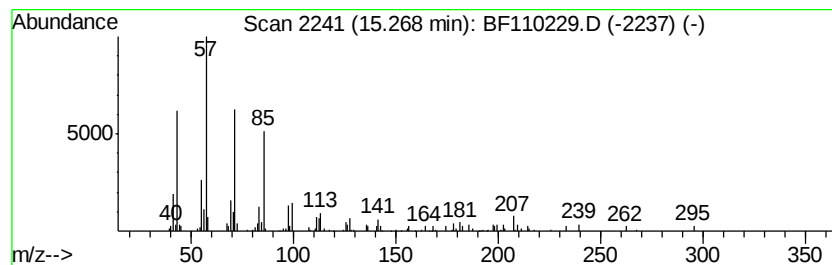
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	3.39 ng	81393	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	87
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
4		Octacosane	394	C28H58	000630-02-4	86
5		Hentriacontane	437	C31H64	000630-04-6	68



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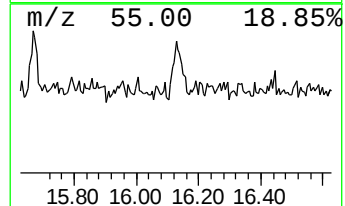
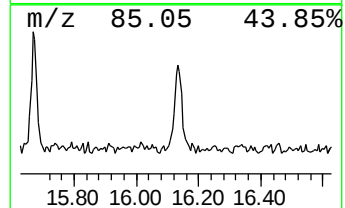
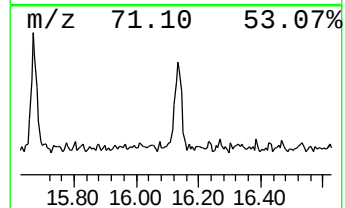
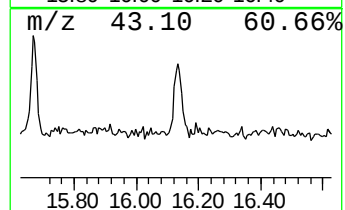
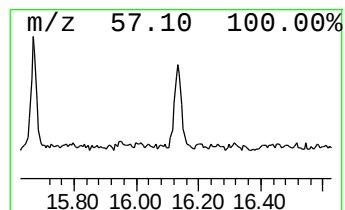
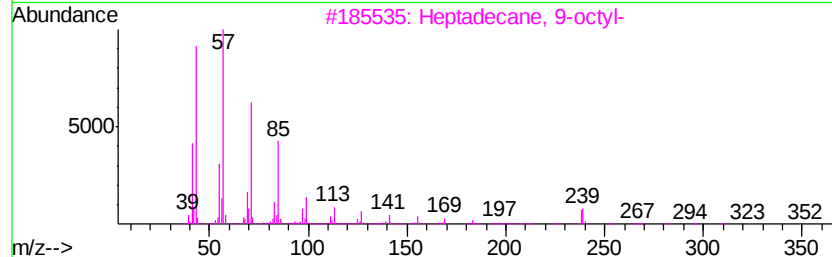
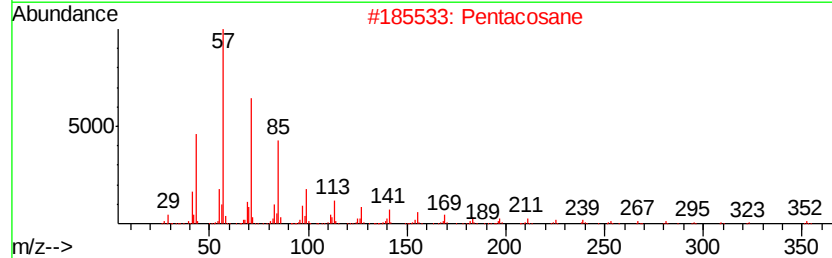
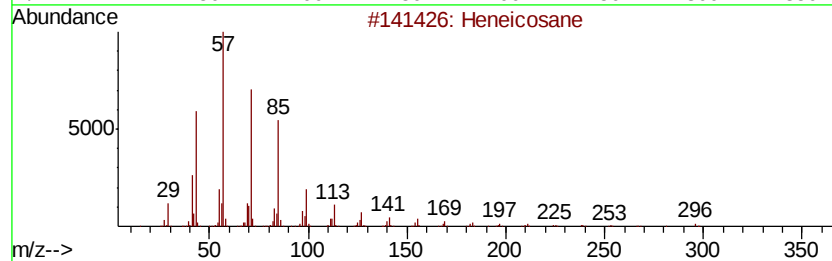
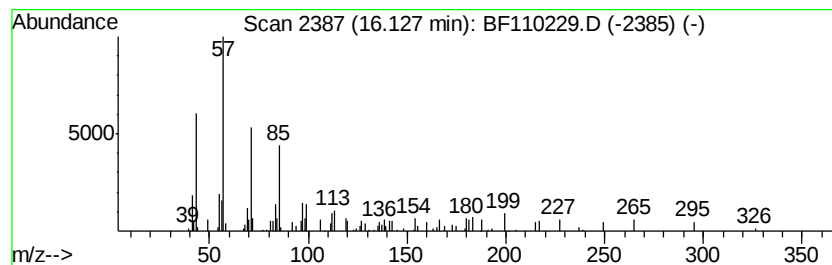
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.26 ng	78206	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	68
2		Pentacosane	352	C25H52	000629-99-2	64
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64
4		Hexacosane	366	C26H54	000630-01-3	59
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102618\
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Misc :
ALS Vial : 24 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.74	6.74	63.6	ng	2499130	1	6.97	785599	20.0
Hexanoic acid, 3,...	7.76	4.7	ng	220321	2	8.25	929733	20.0
Formamide, N,N-di...	8.87	3.1	ng	143110	2	8.25	929733	20.0
unknown11.63	11.63	30.4	ng	1143050	4	11.50	750853	20.0
3-Pyrrolidinecarb...	13.85	11.6	ng	359172	5	14.15	620523	20.0
Tricosyl trifluor...	13.97	2.4	ng	74836	5	14.15	620523	20.0
Tetracosane	14.92	2.5	ng	60450	6	15.68	480095	20.0
Heptadecane, 9-oc...	15.27	3.4	ng	81393	6	15.68	480095	20.0
Heneicosane	16.13	3.3	ng	78206	6	15.68	480095	20.0