

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111919\
 Data File : BF117861.D
 Acq On : 19 Nov 2019 16:03
 Operator : JU
 Sample : K5865-19
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2-(8-10)

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-BF111319.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	2.210	15	21	30	rVB	884281	1210433	19.38%	2.252%
2	5.134	510	518	527	rVB	741602	963347	15.43%	1.792%
3	5.528	580	585	589	rBV	4564594	4802257	76.90%	8.933%
4	6.539	751	757	761	rBV	4954902	5458097	87.41%	10.153%
5	6.681	777	781	785	rBV	5076748	5248007	84.04%	9.762%
6	6.916	817	821	824	rBV	1679319	1318294	21.11%	2.452%
7	7.075	843	848	851	rBV	4763090	4195002	67.18%	7.804%
8	7.475	911	916	919	rBV	3309336	3311633	53.03%	6.160%
9	8.204	1035	1040	1043	rBV	1935118	1740447	27.87%	3.238%
10	9.280	1218	1223	1227	rBV	6388497	6244531	100.00%	11.616%
11	9.675	1286	1290	1293	rBV	703822	560427	8.97%	1.043%
12	9.963	1335	1339	1343	rBV	2259087	2057011	32.94%	3.827%
13	10.757	1469	1474	1477	rBV	4066008	3562287	57.05%	6.627%
14	11.457	1589	1593	1596	rBV	2518203	2048490	32.80%	3.811%
15	11.522	1600	1604	1608	rVB2	100606	89831	1.44%	0.167%
16	11.974	1678	1681	1685	rBV	109763	120504	1.93%	0.224%
17	12.763	1811	1815	1821	rBV	64906	88166	1.41%	0.164%
18	13.051	1859	1864	1867	rBV	6323861	5964351	95.51%	11.095%
19	14.104	2036	2043	2047	rBV	1770555	1603187	25.67%	2.982%
20	14.268	2067	2071	2077	rBV	109178	118295	1.89%	0.220%
21	14.574	2119	2123	2127	rBV	176530	173629	2.78%	0.323%
22	14.892	2173	2177	2182	rVB	232602	253244	4.06%	0.471%
23	14.968	2186	2190	2197	rVV	222299	233302	3.74%	0.434%
24	15.245	2233	2237	2243	rBV	237113	268571	4.30%	0.500%
25	15.609	2294	2299	2303	rBV	1138203	1430574	22.91%	2.661%
26	15.645	2303	2305	2310	rVB	210375	235636	3.77%	0.438%
27	16.104	2378	2383	2388	rBV	137872	214509	3.44%	0.399%
28	16.639	2469	2474	2481	rVB	85667	148578	2.38%	0.276%
29	17.268	2575	2581	2589	rVB4	34947	94318	1.51%	0.175%

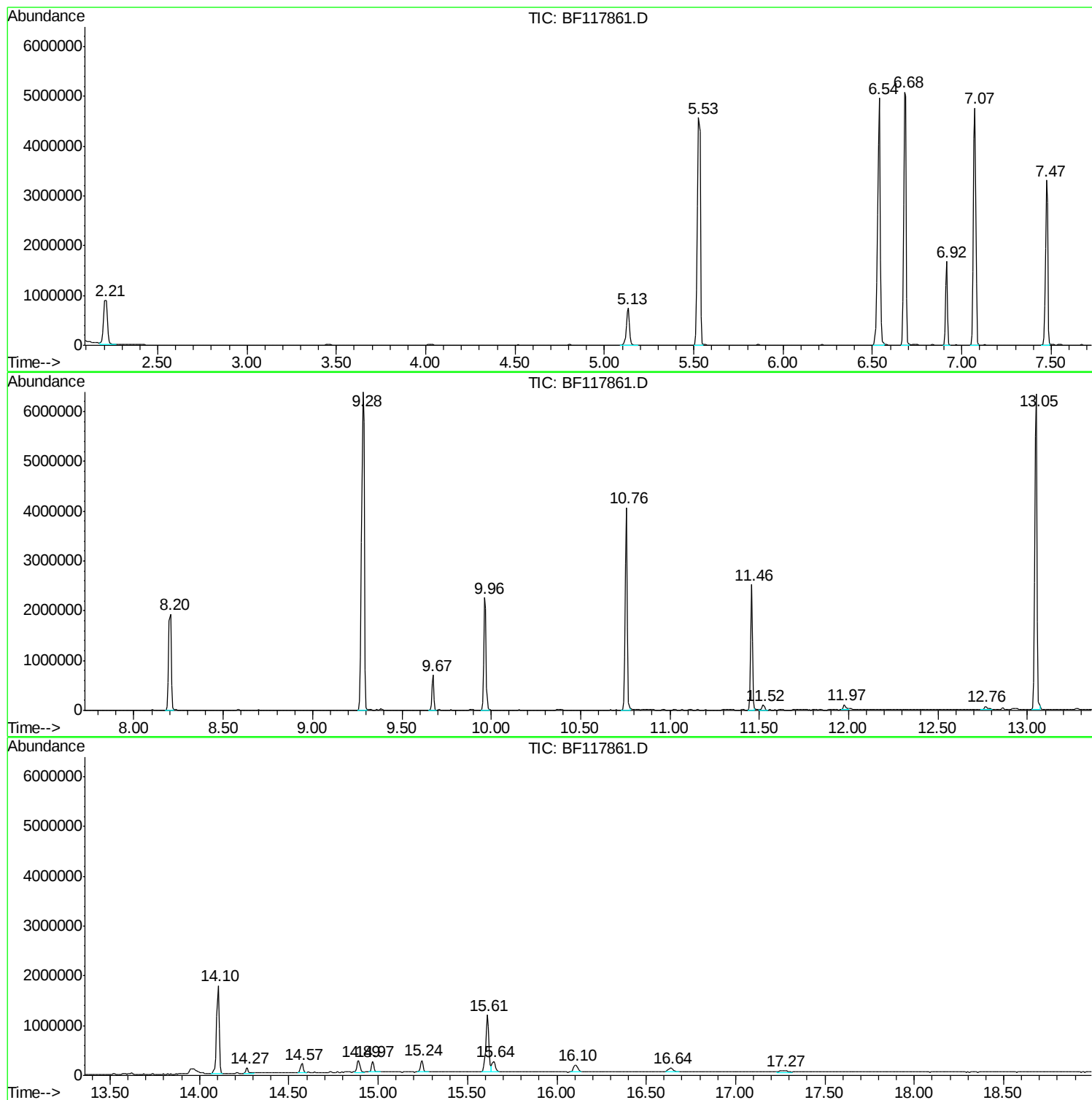
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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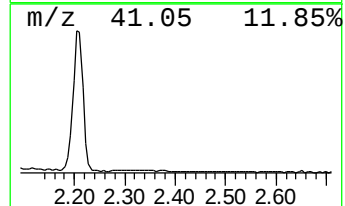
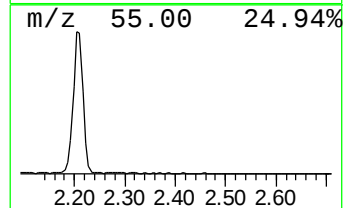
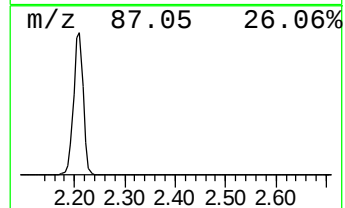
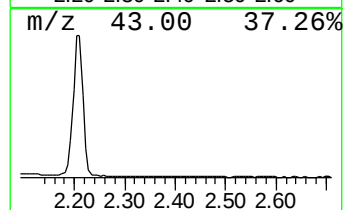
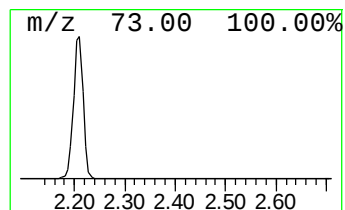
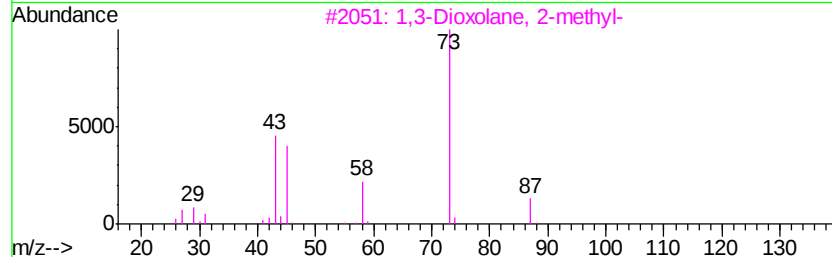
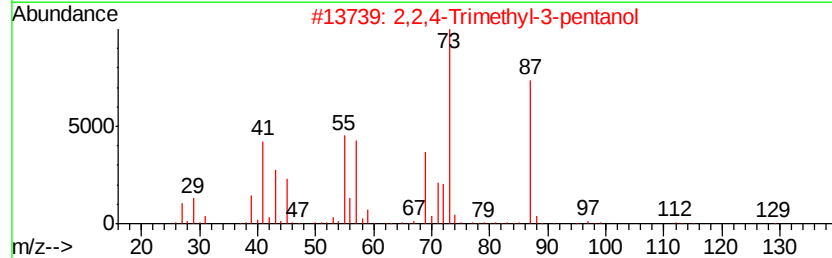
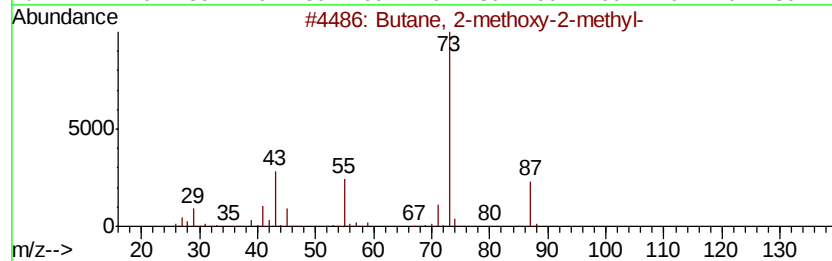
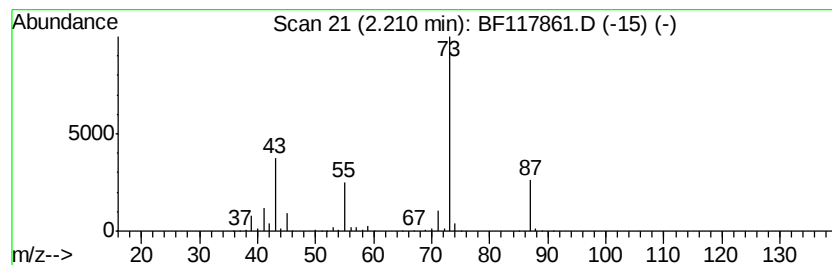
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	18.36 ng	1210430	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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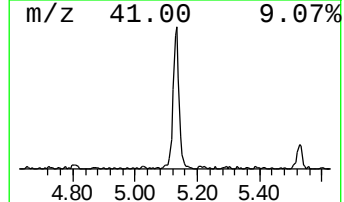
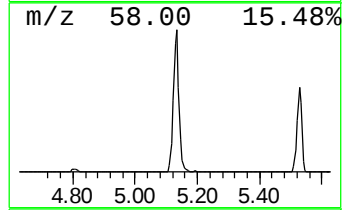
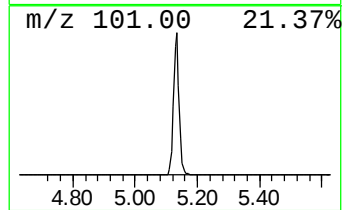
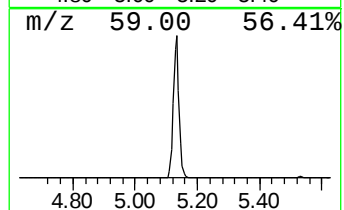
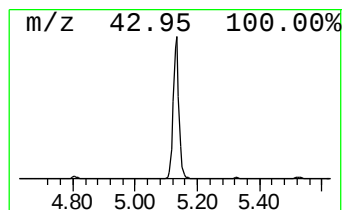
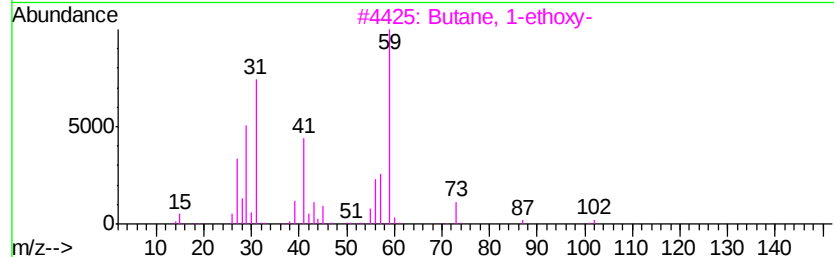
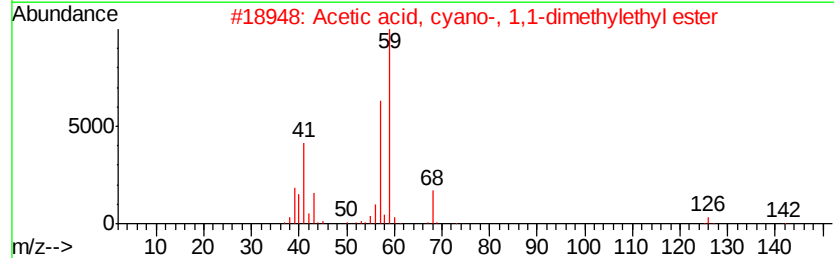
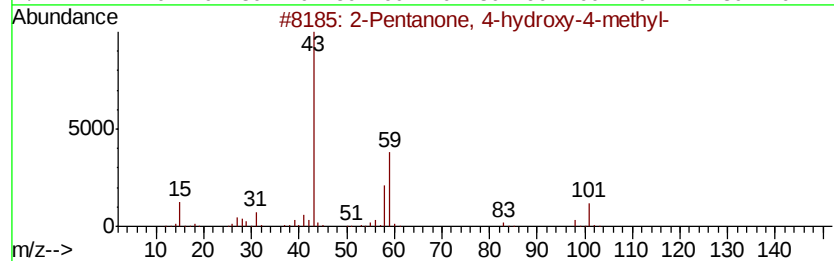
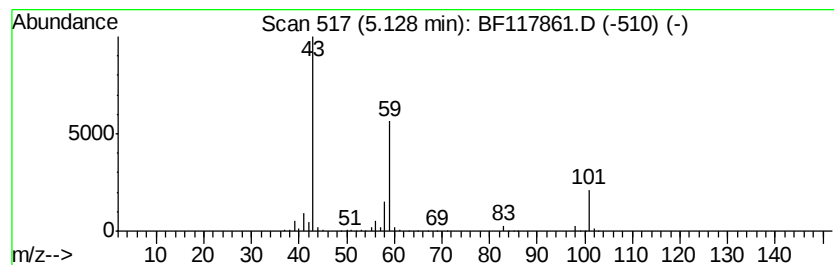
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	14.62 ng	963347	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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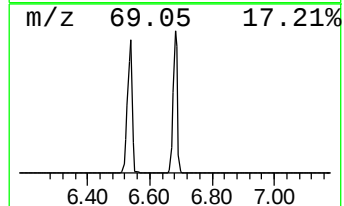
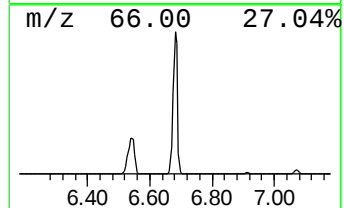
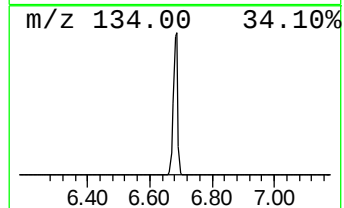
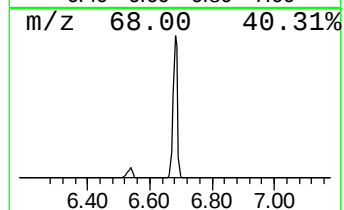
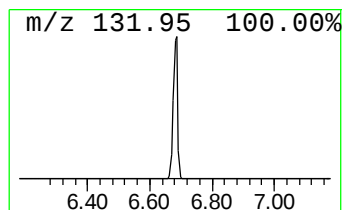
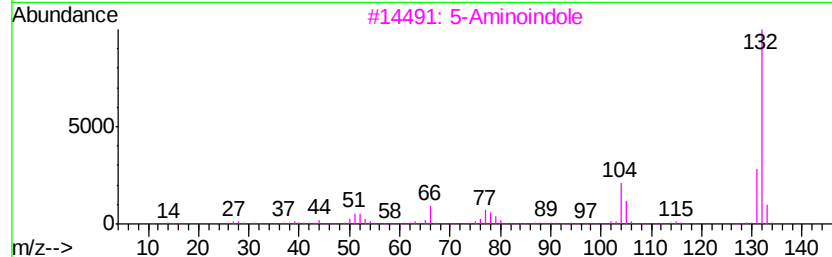
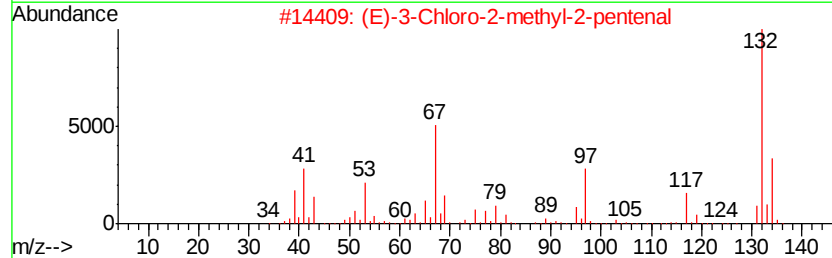
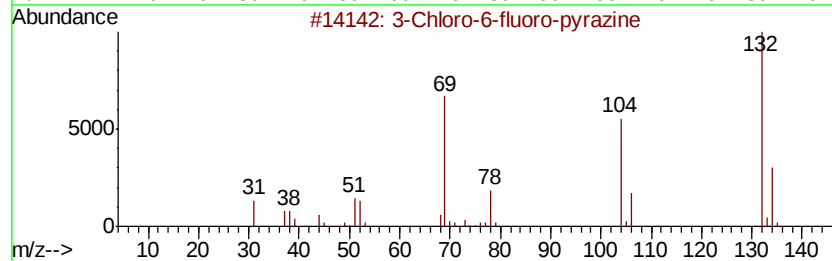
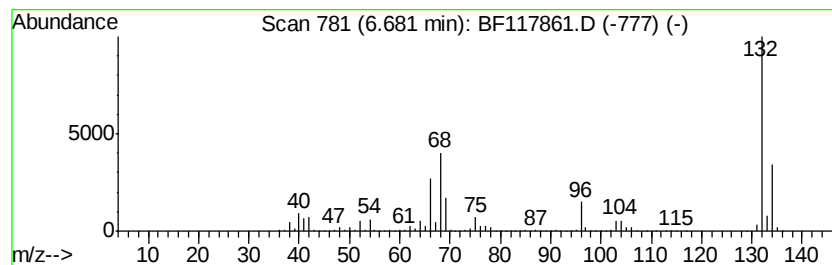
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	79.62 ng	5248010	1,4-Dichlorobenzene-d4	6.92

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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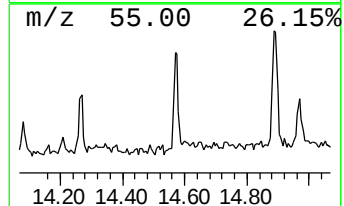
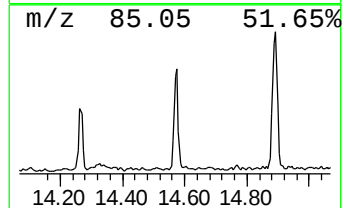
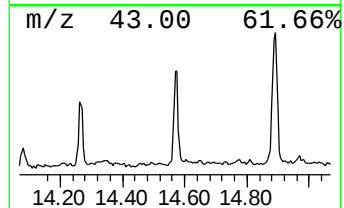
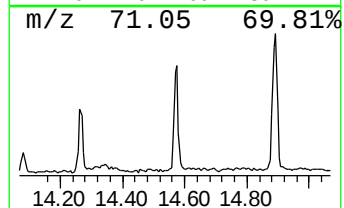
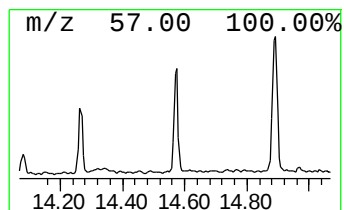
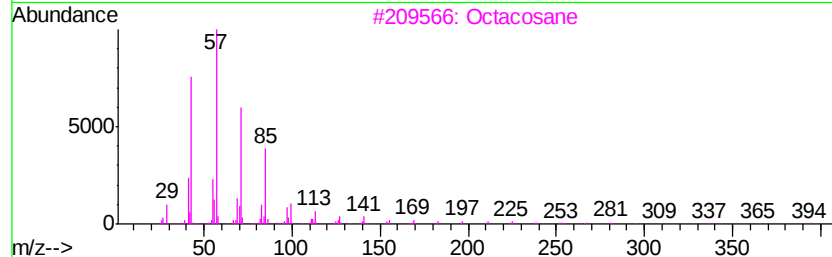
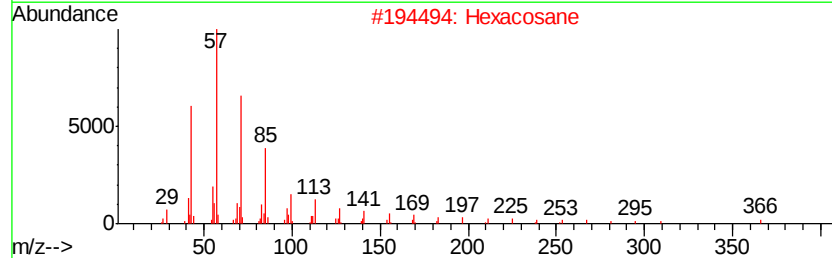
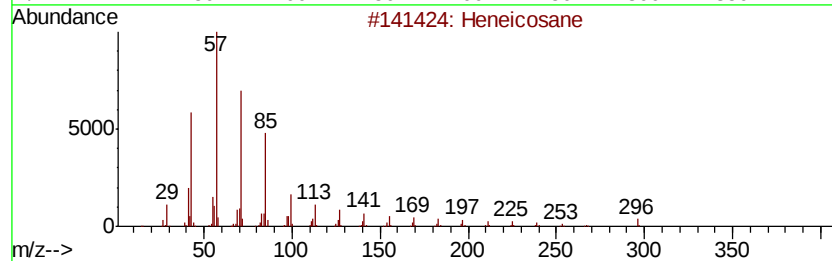
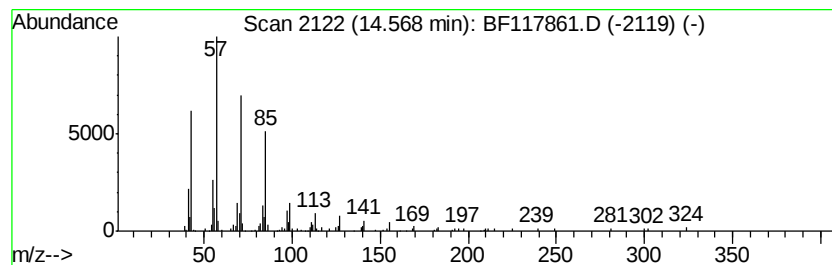
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Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.17 ng	173629	Chrysene-d12	14.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	87
3	Octacosane		394	C28H58	000630-02-4	87
4	Octadecane		254	C18H38	000593-45-3	87
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87



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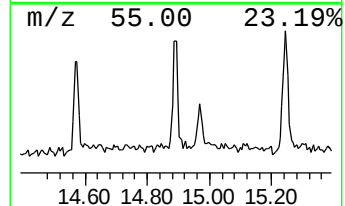
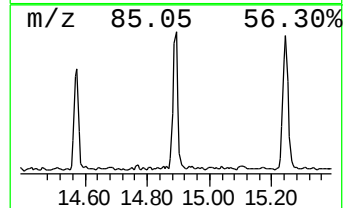
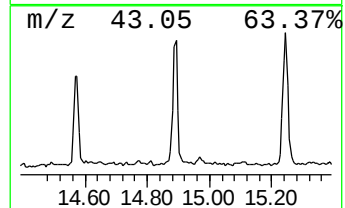
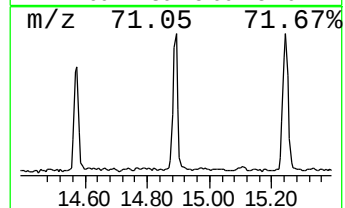
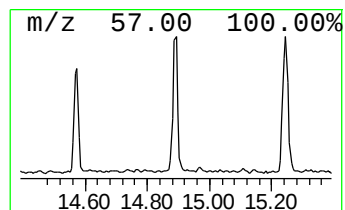
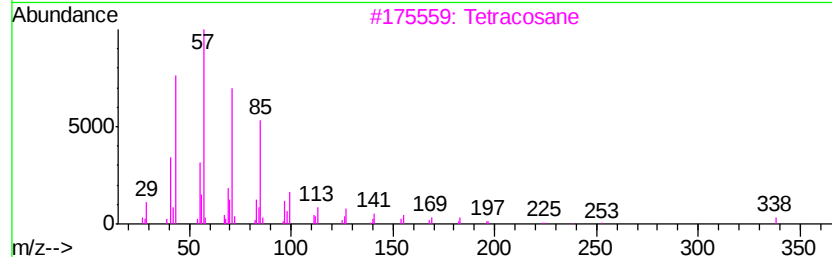
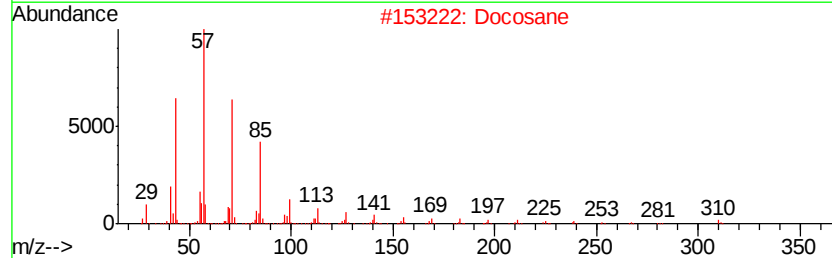
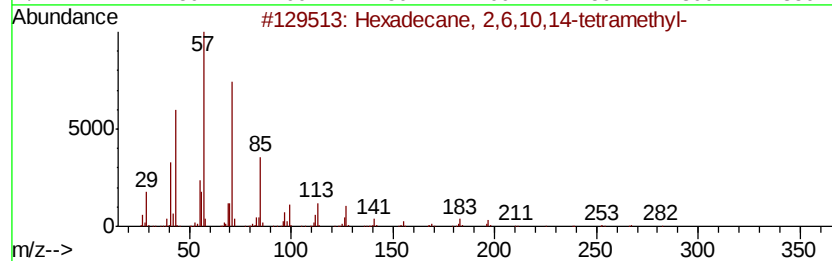
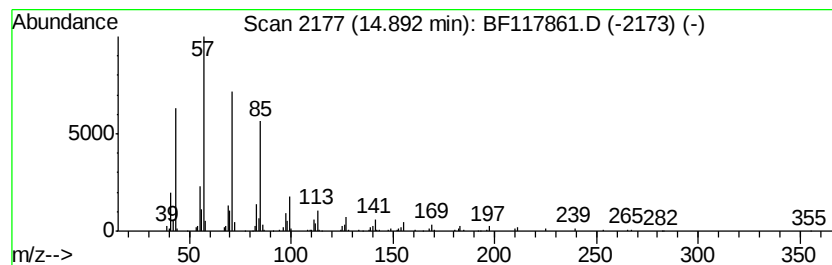
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	3.54 ng	253244	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	93
2		Docosane	310	C22H46	000629-97-0	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Heneicosane	296	C21H44	000629-94-7	91



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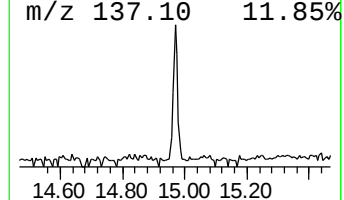
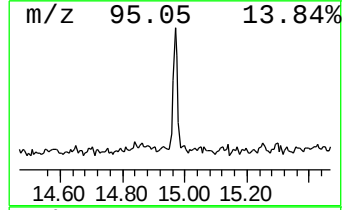
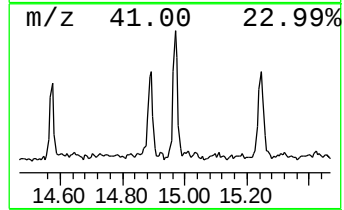
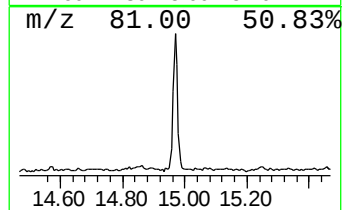
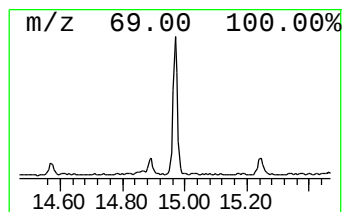
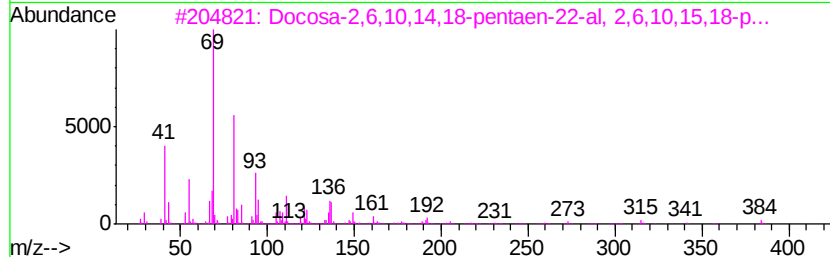
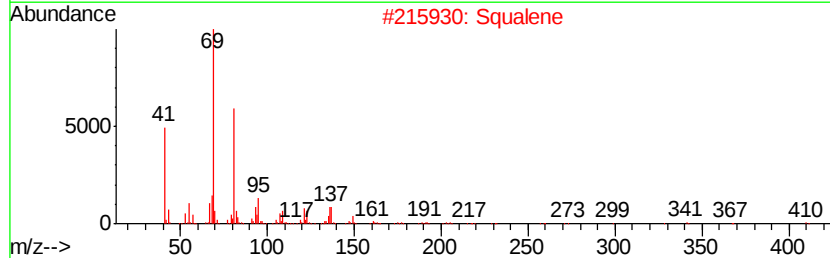
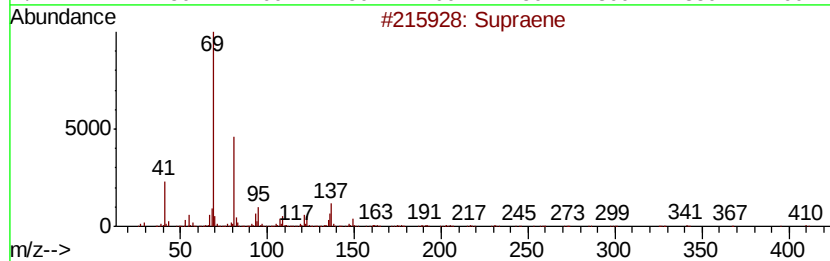
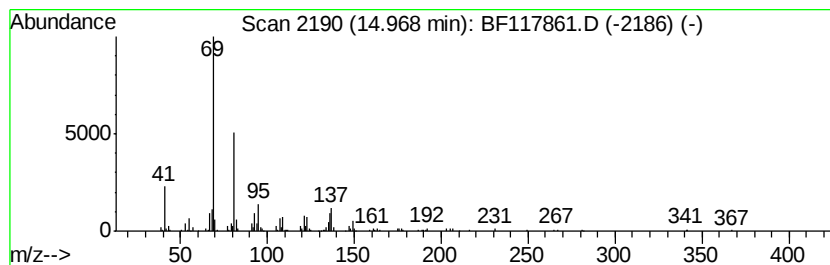
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	3.26 ng	233302	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	83
5		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117861.D
Acq On : 19 Nov 2019 16:03
Operator : JU
Sample : K5865-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-(8-10)

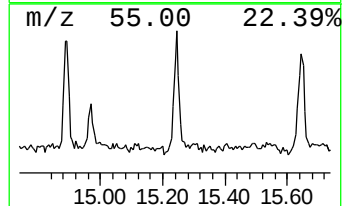
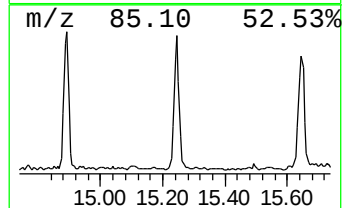
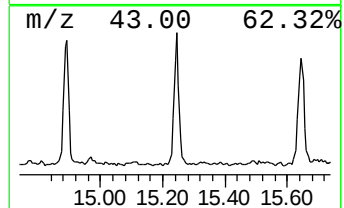
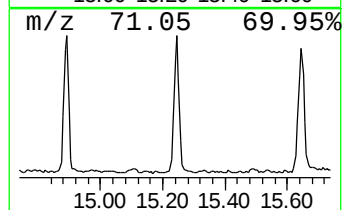
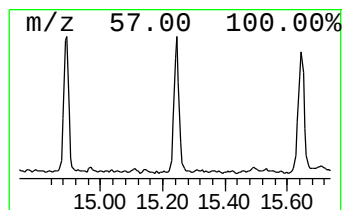
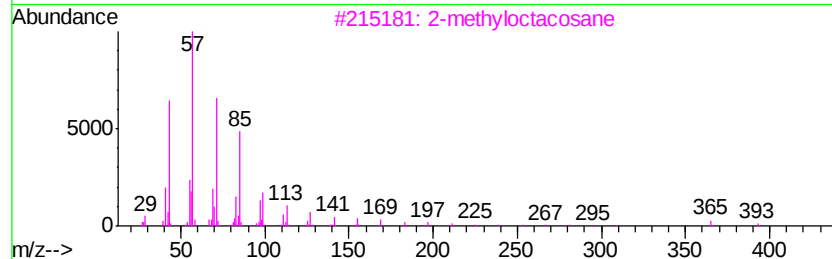
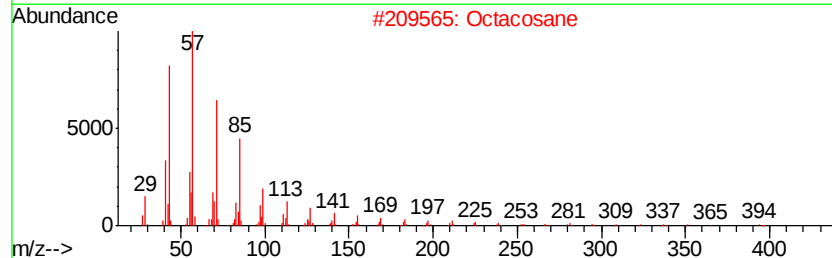
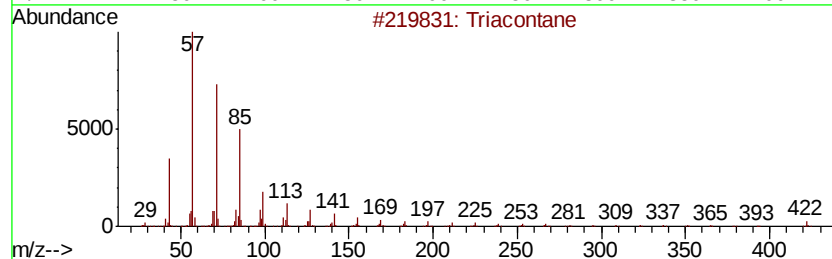
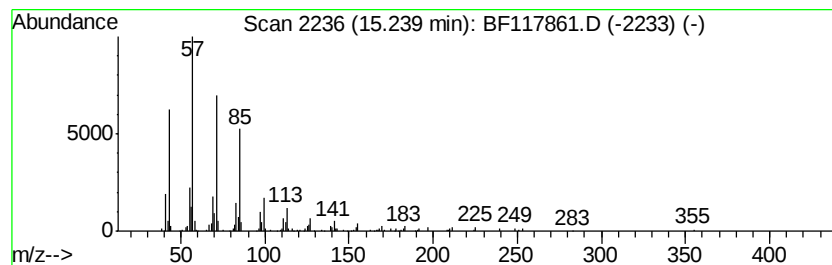
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	3.75 ng	268571	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Octacosane	394	C28H58	000630-02-4	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117861.D
Acq On : 19 Nov 2019 16:03
Operator : JU
Sample : K5865-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-(8-10)

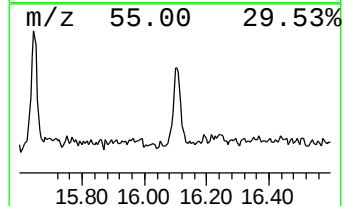
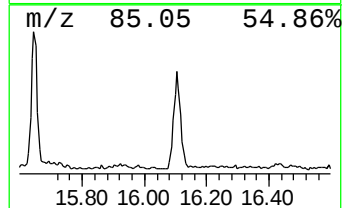
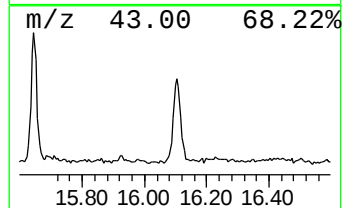
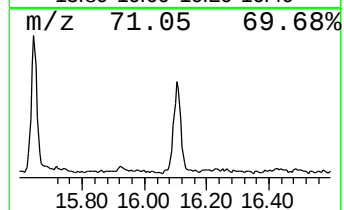
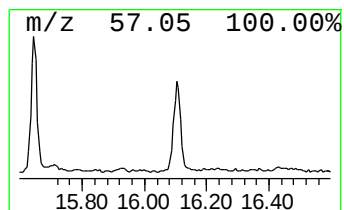
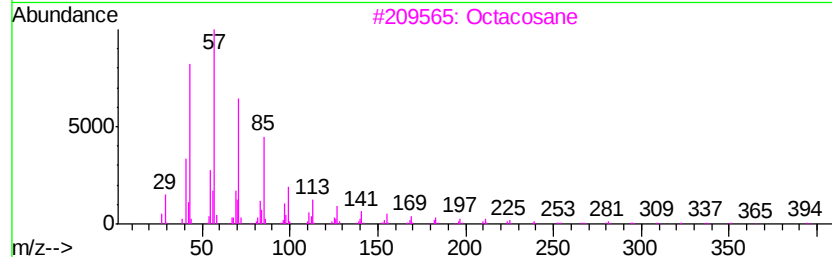
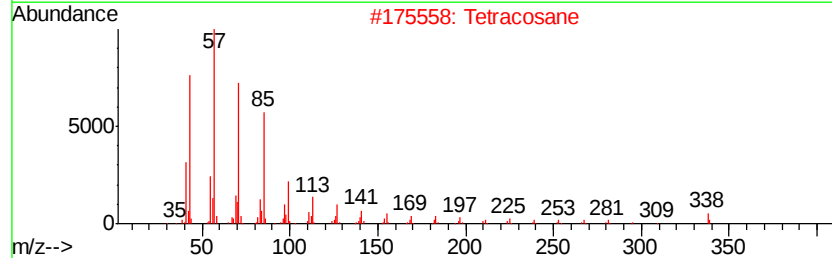
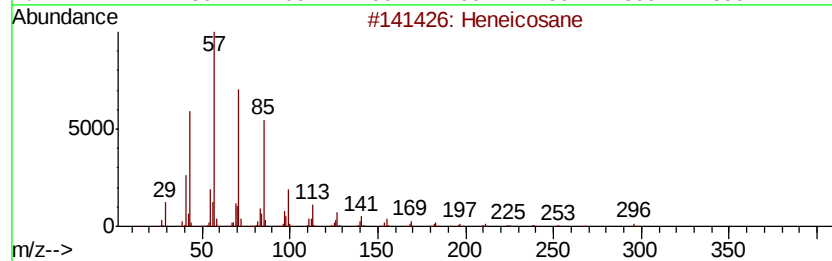
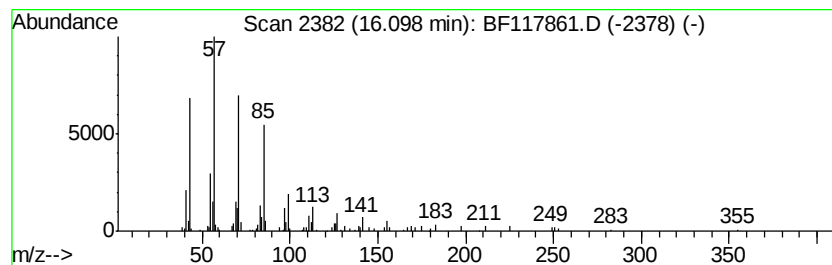
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	3.00 ng	214509	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117861.D
Acq On : 19 Nov 2019 16:03
Operator : JU
Sample : K5865-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-(8-10)

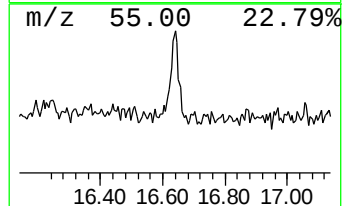
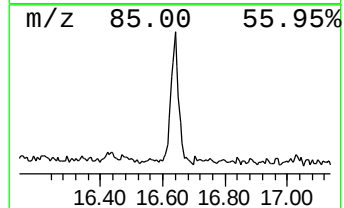
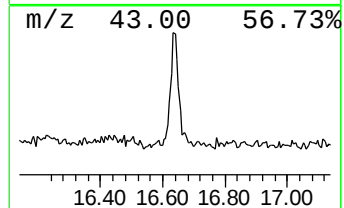
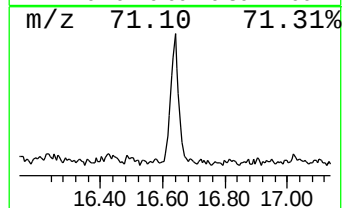
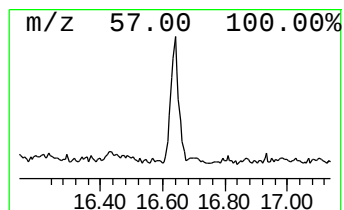
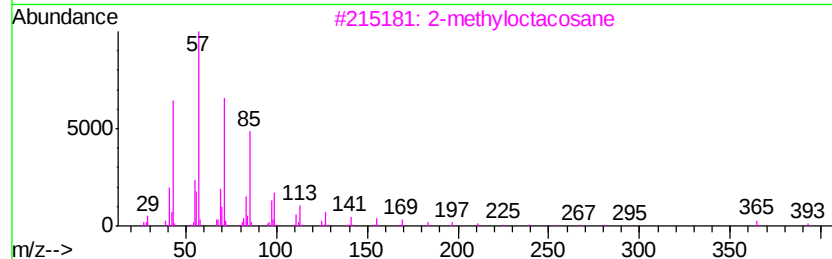
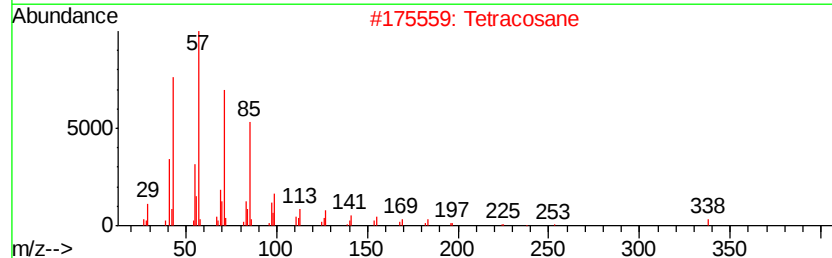
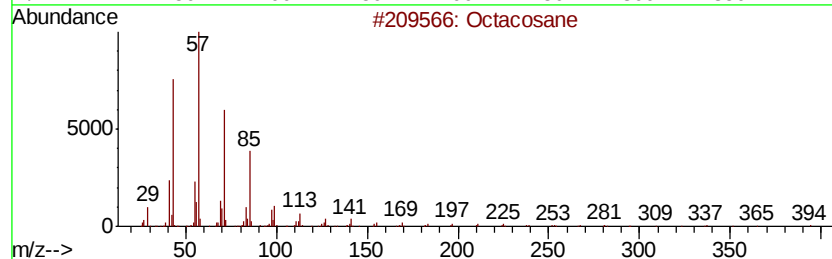
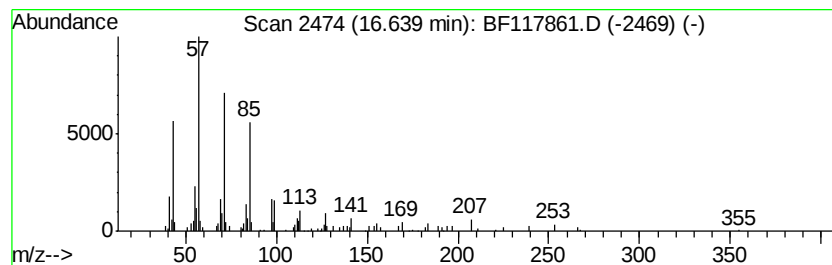
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	2.08 ng	148578	Perylene-d12	15.61

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Tetracosane	338	C24H50	000646-31-1	90
3			2-methyloctacosane	408	C29H60	1000376-72-8	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111919\
Data File : BF117861.D
Acq On : 19 Nov 2019 16:03
Operator : JU
Sample : K5865-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-(8-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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
Butane, 2-methoxy...	2.21	18.4	ng	1210430	1	6.92	1318290	20.0
2-Pentanone, 4-hy...	5.13	14.6	ng	963347	1	6.92	1318290	20.0
unknown6.68	6.68	79.6	ng	5248010	1	6.92	1318290	20.0
Heneicosane	14.57	2.2	ng	173629	5	14.10	1603190	20.0
Hexadecane, 2,6,1...	14.89	3.5	ng	253244	6	15.61	1430570	20.0
Supraene	14.97	3.3	ng	233302	6	15.61	1430570	20.0
Triacontane	15.24	3.8	ng	268571	6	15.61	1430570	20.0
Tetracosane	16.10	3.0	ng	214509	6	15.61	1430570	20.0
Octacosane	16.64	2.1	ng	148578	6	15.61	1430570	20.0