

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102120\
 Data File : BF122052.D
 Acq On : 21 Oct 2020 13:39
 Operator : JU/CG
 Sample : L4309-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OWLS-HEAD-BH-04-B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.269	367	371	389	rBV	539434	728295	25.39%	3.567%
2	4.922	478	482	495	rBV	222898	298355	10.40%	1.461%
3	5.345	551	554	577	rBV	1391990	1596570	55.65%	7.819%
4	6.375	725	729	751	rBV	1833629	1893260	66.00%	9.272%
5	6.722	785	788	798	rVB	751949	657235	22.91%	3.219%
6	7.292	881	885	898	rBV	1482491	1367155	47.66%	6.696%
7	8.010	1003	1007	1024	rBV	909467	884149	30.82%	4.330%
8	9.080	1185	1189	1192	rBV	2697650	2296070	80.04%	11.245%
9	9.480	1253	1257	1264	rBV	150814	136140	4.75%	0.667%
10	9.757	1300	1304	1314	rVB	1185892	1022345	35.64%	5.007%
11	10.545	1435	1438	1455	rBV	947823	1028847	35.86%	5.039%
12	11.245	1553	1557	1565	rBV	1166027	1125957	39.25%	5.514%
13	11.768	1638	1646	1653	rBV2	74673	106468	3.71%	0.521%
14	12.204	1716	1720	1727	rBV	29373	29417	1.03%	0.144%
15	12.457	1760	1763	1769	rBV	140284	120891	4.21%	0.592%
16	12.686	1797	1802	1805	rVB	117320	121793	4.25%	0.596%
17	12.827	1821	1826	1829	rBV	2894414	2868706	100.00%	14.050%
18	13.115	1872	1875	1890	rVB7	35446	104763	3.65%	0.513%
19	13.721	1970	1978	1995	rBV4	241103	528327	18.42%	2.587%
20	13.880	2001	2005	2008	rBV	1248275	1181868	41.20%	5.788%
21	13.904	2008	2009	2013	rVB	72581	56497	1.97%	0.277%
22	13.992	2014	2024	2028	rBV	39963	123085	4.29%	0.603%
23	14.027	2028	2030	2040	rVB4	41021	82320	2.87%	0.403%
24	14.274	2067	2072	2073	rBV2	25206	30653	1.07%	0.150%
25	14.333	2079	2082	2085	rVB2	46347	51503	1.80%	0.252%
26	14.633	2128	2133	2137	rVB	66742	75605	2.64%	0.370%
27	14.698	2139	2144	2148	rVV	176293	206567	7.20%	1.012%
28	14.904	2175	2179	2182	rBV	63087	90775	3.16%	0.445%
29	14.945	2183	2186	2191	rVV	92445	118198	4.12%	0.579%
30	15.015	2194	2198	2204	rBV2	18648	32484	1.13%	0.159%
31	15.192	2225	2228	2234	rVB	32587	40465	1.41%	0.198%
32	15.251	2235	2238	2242	rBV	42796	49761	1.73%	0.244%
33	15.309	2243	2248	2256	rBV	819603	1070753	37.33%	5.244%
34	15.709	2311	2316	2321	rBV	64138	92483	3.22%	0.453%
35	15.792	2324	2330	2332	rBV7	24895	50958	1.78%	0.250%
36	16.174	2390	2395	2400	rVB	42781	70965	2.47%	0.348%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.721	2482	2488	2495	rVB4	37079	78864	2.75%	0.386%
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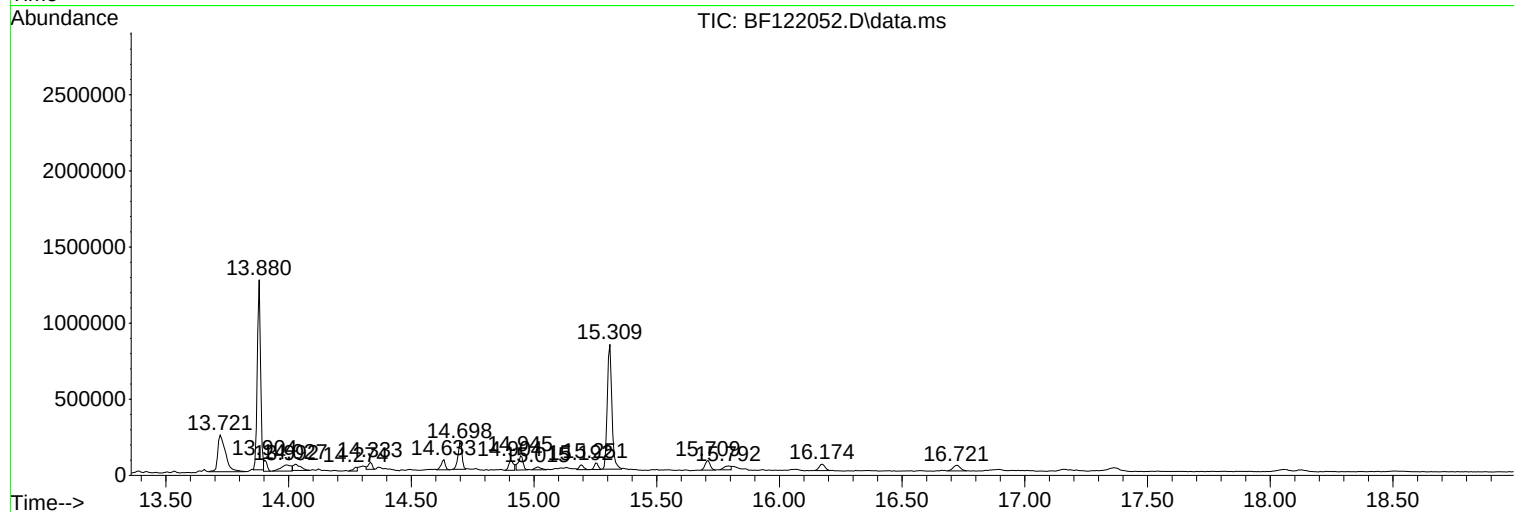
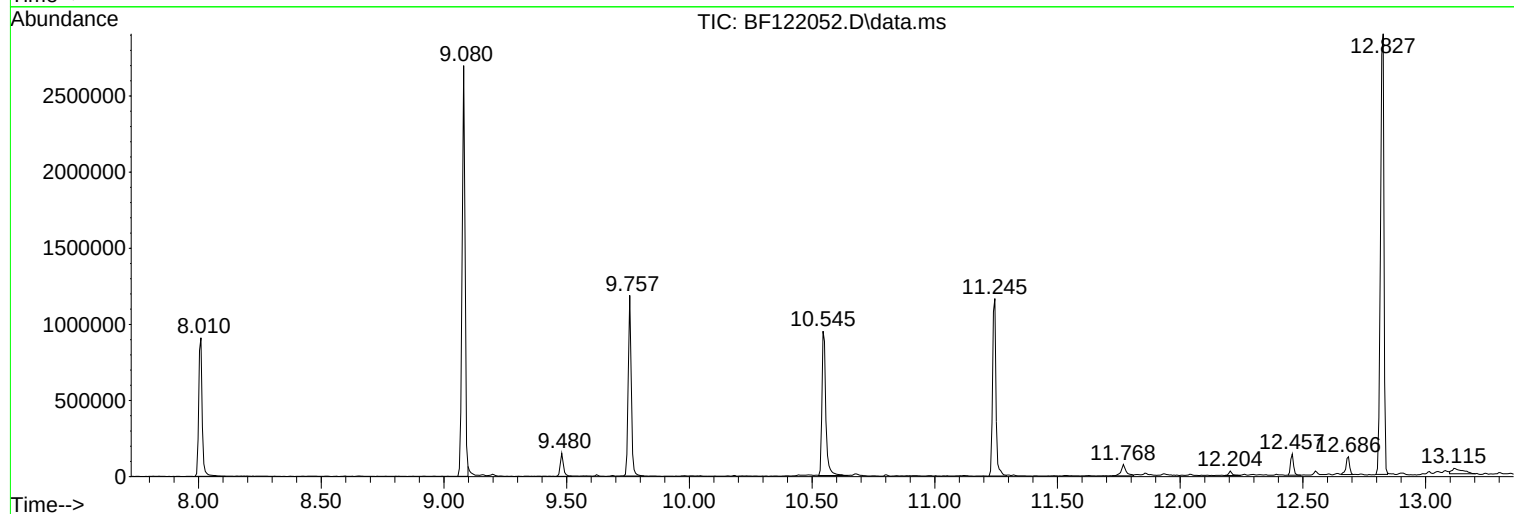
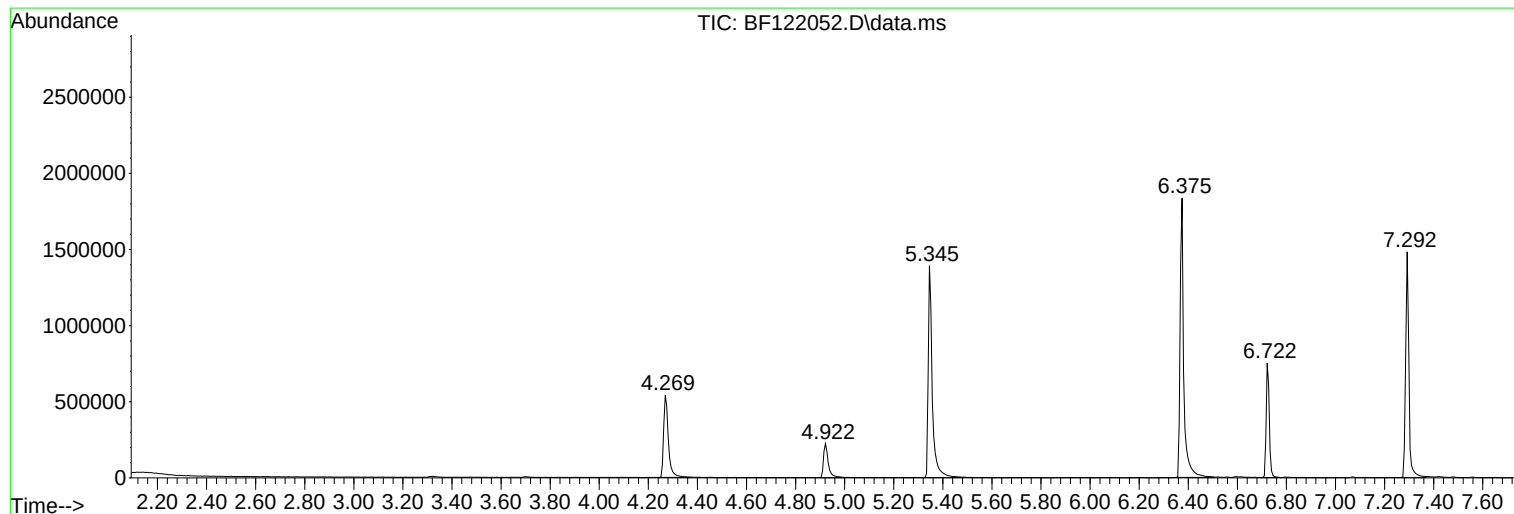
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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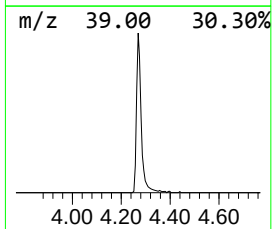
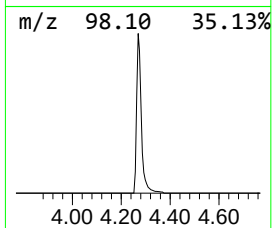
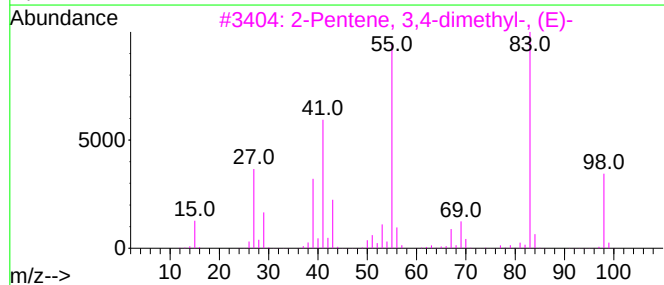
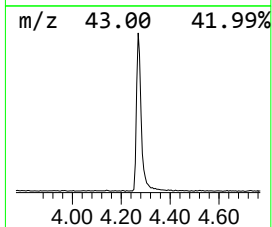
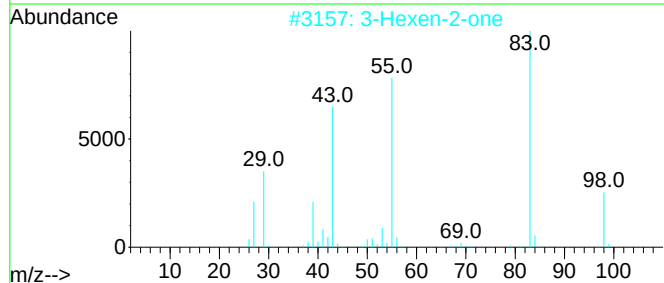
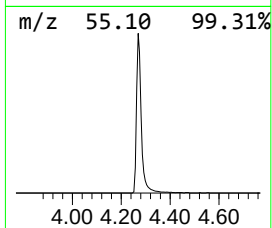
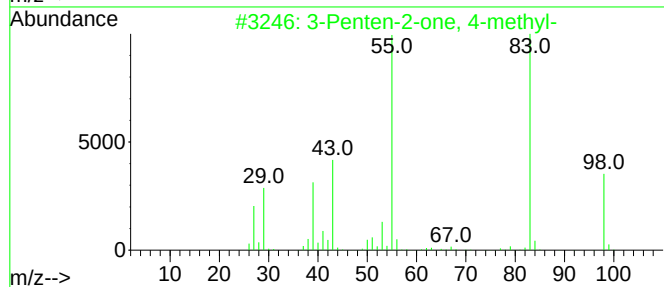
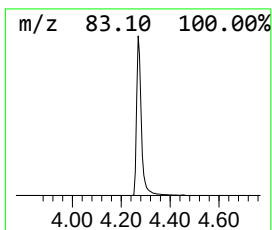
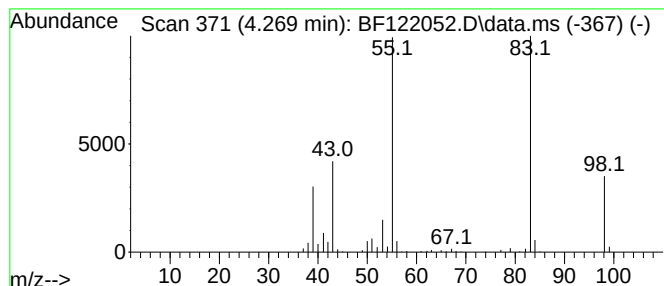
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.269	22.16 ng	728295	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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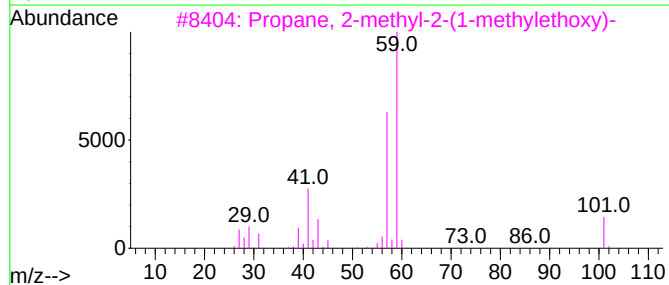
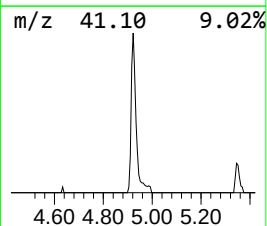
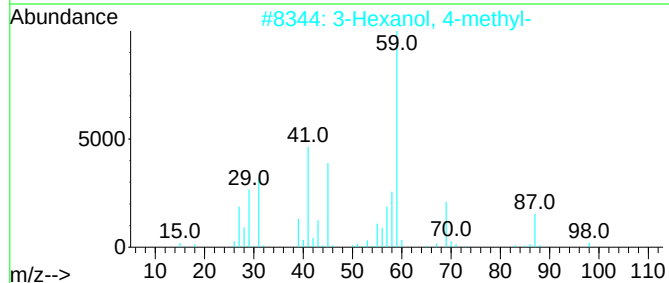
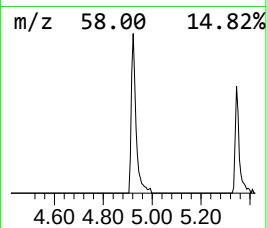
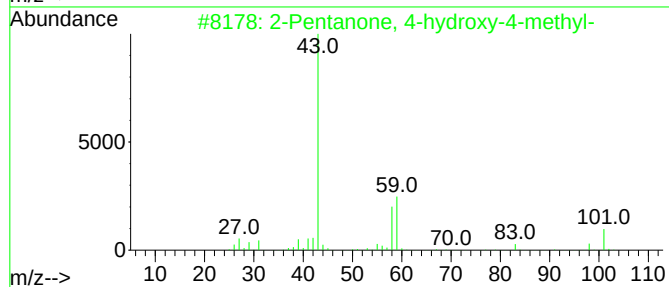
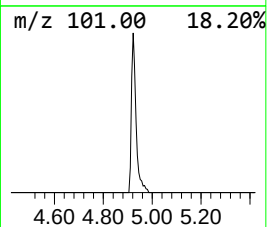
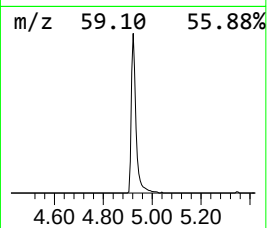
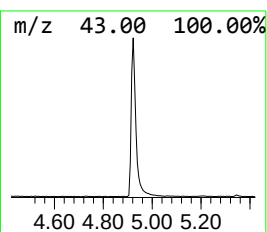
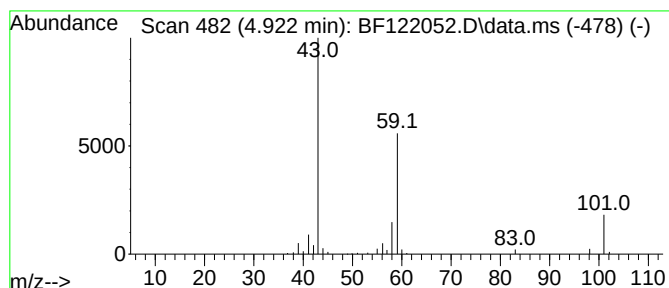
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	9.08 ng	298355	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
4	3-Hexanol	102	C6H14O	000623-37-0	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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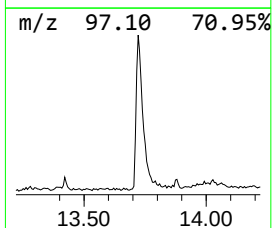
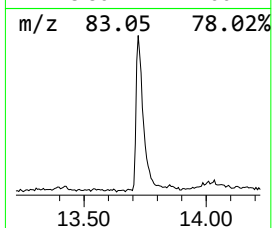
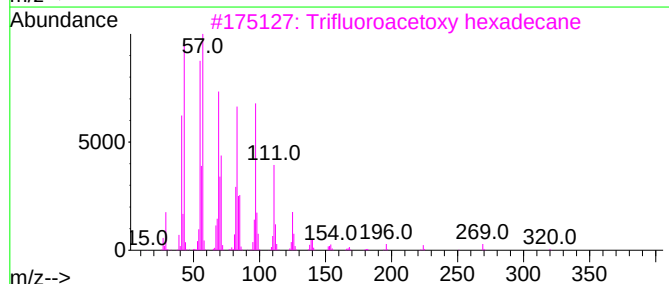
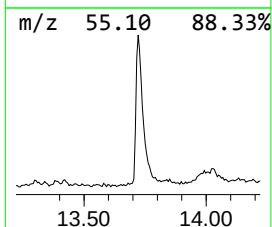
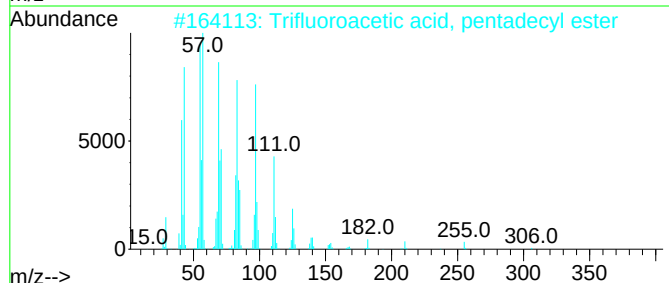
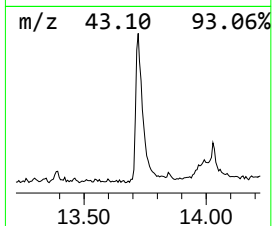
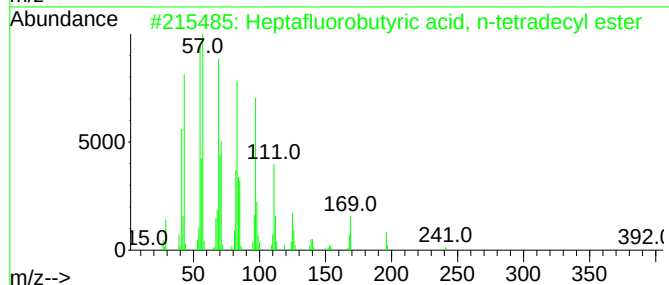
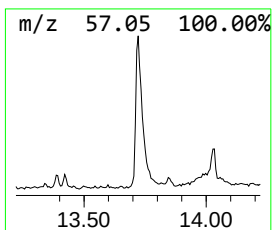
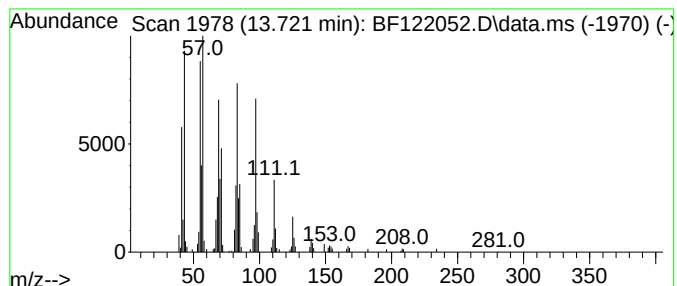
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.721	8.94 ng	528327	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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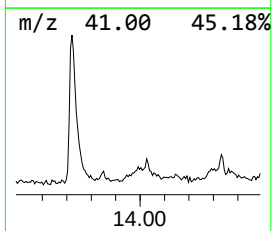
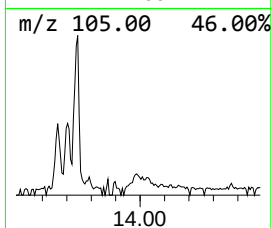
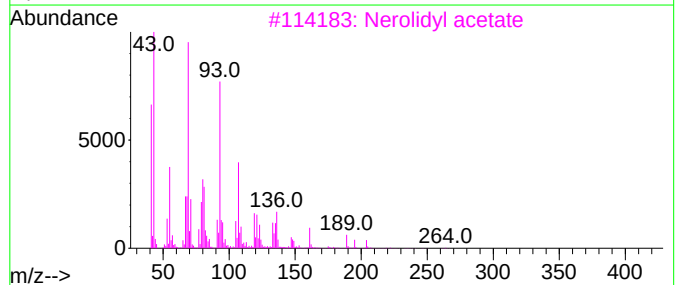
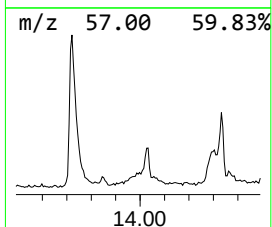
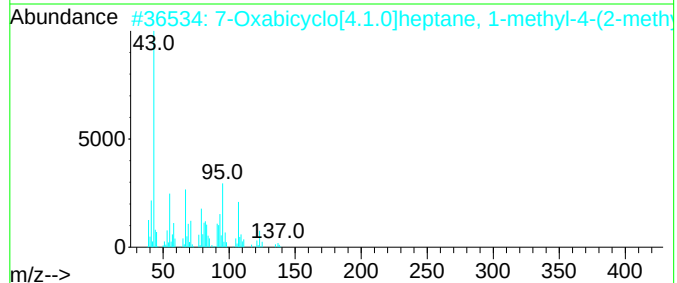
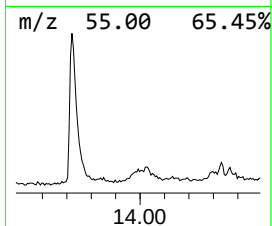
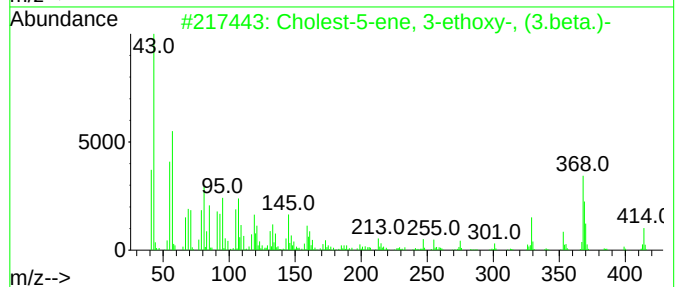
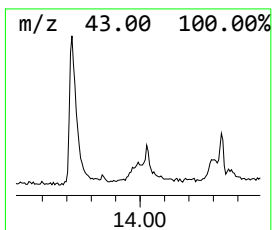
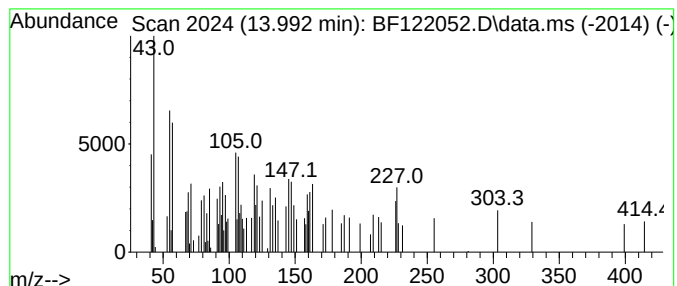
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.99 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	2.08 ng	123085	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	11
2			7-Oxabicyclo[4.1.0]heptane, 1-me...	168	C10H16O2	000096-08-2	10
3			Nerolidyl acetate	264	C17H28O2	002306-78-7	10
4			Benzofuran, 7-(2,4-dinitrophenox...	374	C18H18N2O7	062059-46-5	10
5			9,19-Cyclolanostan-3-ol, acetate...	470	C32H54O2	004575-74-0	10



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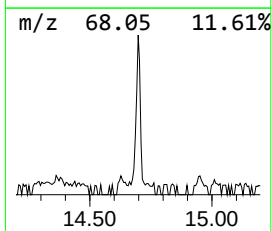
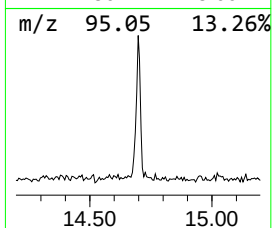
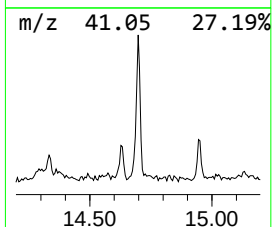
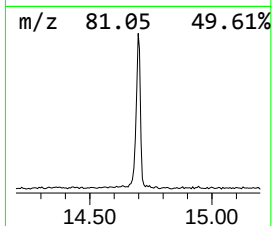
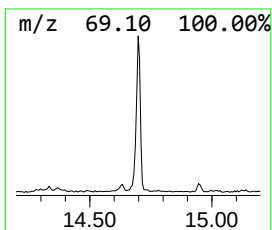
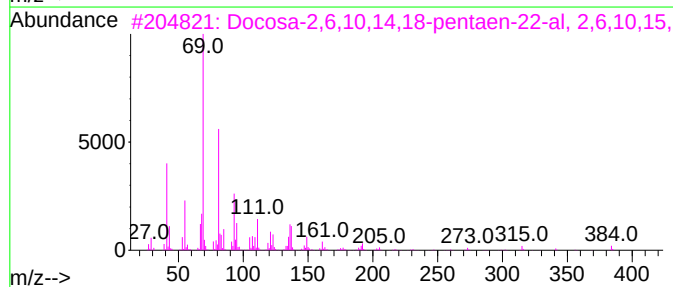
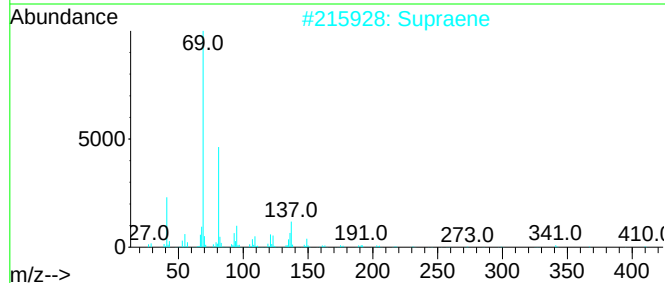
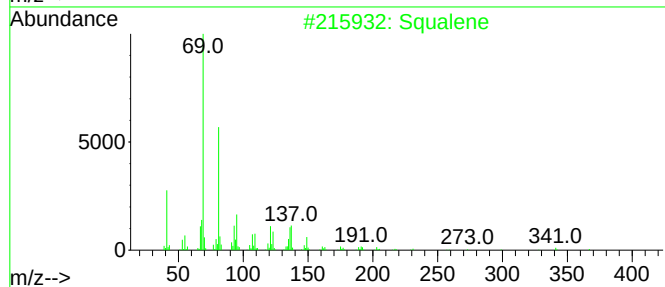
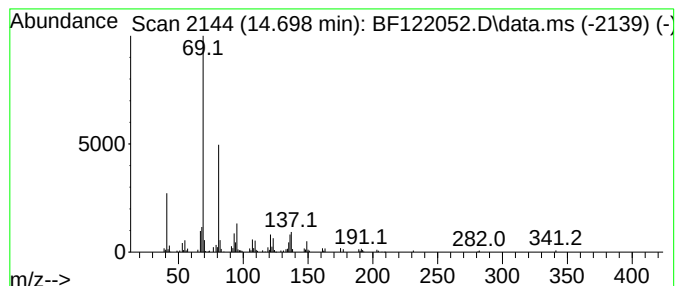
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.698	3.86 ng	206567	Perylene-d12	15.309

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	94
2			Supraene	410	C30H50	007683-64-9	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4			2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102120\
Data File : BF122052.D
Acq On : 21 Oct 2020 13:39
Operator : JU/CG
Sample : L4309-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OWLS-HEAD-BH-04-B

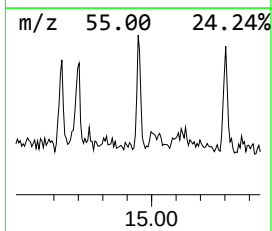
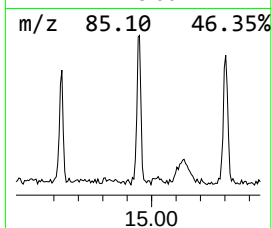
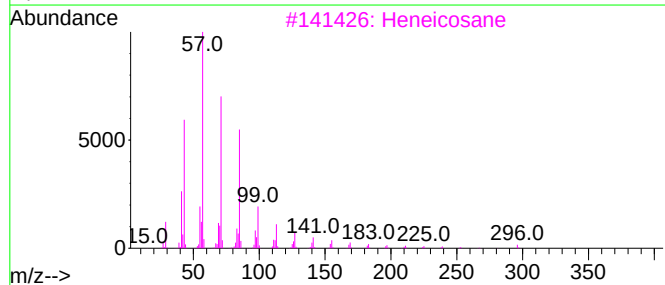
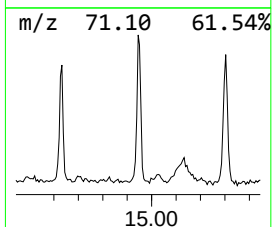
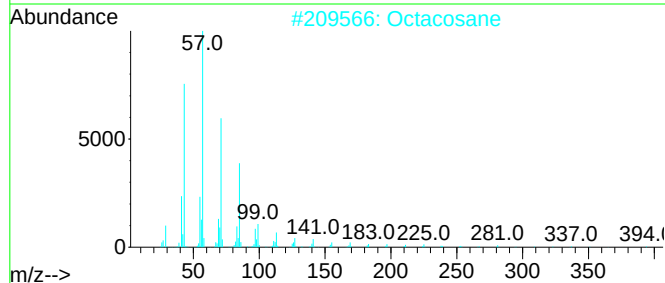
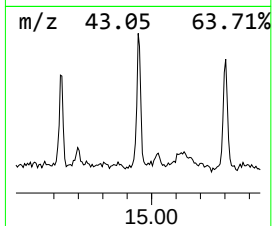
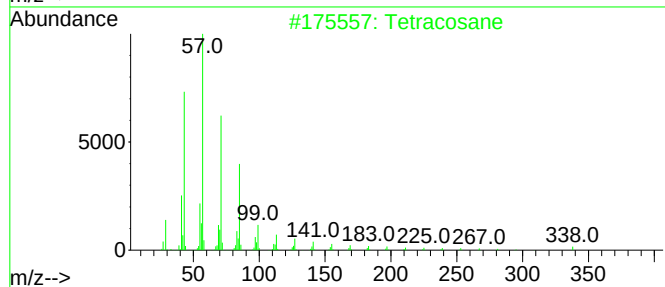
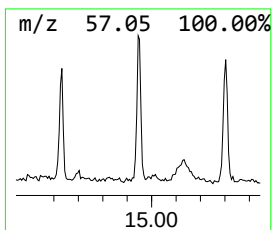
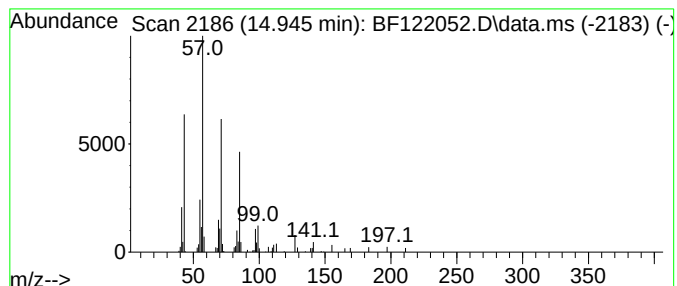
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.945	2.21 ng	118198	Perylene-d12	15.309

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Heneicosane	296	C21H44	000629-94-7	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102120\
Data File : BF122052.D
Acq On : 21 Oct 2020 13:39
Operator : JU/CG
Sample : L4309-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OWLS-HEAD-BH-04-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
3-Penten-2-one,...	4.269	22.2	ng	728295	1	6.722	657235	20.0
2-Pentanone, 4-...	4.922	9.1	ng	298355	1	6.722	657235	20.0
Heptafluorobuty...	13.721	8.9	ng	528327	5	13.880	1181870	20.0
unknown13.99	13.992	2.1	ng	123085	5	13.880	1181870	20.0
Squalene	14.698	3.9	ng	206567	6	15.309	1070750	20.0
Tetracosane	14.945	2.2	ng	118198	6	15.309	1070750	20.0