

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091520\
 Data File : BF121576.D
 Acq On : 15 Sep 2020 14:27
 Operator : JU/CG
 Sample : L3998-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-EF-01-TEST1-ABCD-B

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-BF091020.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	2.134	4	8	14	rVB	253768	330950	5.55%	0.795%
2	5.063	501	506	513	rVB	90404	124009	2.08%	0.298%
3	5.463	569	574	577	rBV	4337148	4128017	69.29%	9.911%
4	6.469	740	745	764	rVB	3892878	4591160	77.06%	11.022%
5	6.663	775	778	789	rBV	96429	106623	1.79%	0.256%
6	6.828	803	806	810	rBV	1372516	1223295	20.53%	2.937%
7	7.392	897	902	905	rBV	2937683	3081901	51.73%	7.399%
8	8.116	1020	1025	1028	rBV	1731287	1624511	27.27%	3.900%
9	9.192	1202	1208	1211	rBV	5224302	5191780	87.14%	12.464%
10	9.580	1270	1274	1278	rBV	578132	471499	7.91%	1.132%
11	9.869	1317	1323	1326	rBV	2014780	1928371	32.37%	4.630%
12	10.657	1451	1457	1460	rBV	3736714	3540923	59.43%	8.501%
13	11.351	1570	1575	1578	rBV	2374018	2034943	34.16%	4.885%
14	11.880	1661	1665	1677	rBV	776874	770652	12.94%	1.850%
15	12.563	1777	1781	1786	rBV	66276	75665	1.27%	0.182%
16	12.663	1794	1798	1805	rBV	197575	208832	3.51%	0.501%
17	12.939	1838	1845	1848	rBV	6024654	5957756	100.00%	14.303%
18	13.162	1878	1883	1890	rBV4	56184	91609	1.54%	0.220%
19	13.509	1936	1942	1944	rBV2	73475	77326	1.30%	0.186%
20	13.833	1993	1997	2010	rBV	1006964	1386181	23.27%	3.328%
21	13.986	2018	2023	2026	rBV	2144018	1932763	32.44%	4.640%
22	14.151	2048	2051	2054	rBV	97810	107763	1.81%	0.259%
23	14.457	2100	2103	2105	rBV	128989	123385	2.07%	0.296%
24	14.762	2152	2155	2158	rVB	89948	82084	1.38%	0.197%
25	14.839	2164	2168	2171	rVB	154464	162381	2.73%	0.390%
26	15.098	2208	2212	2216	rBV	111336	120333	2.02%	0.289%
27	15.439	2265	2270	2274	rBV	1163597	1437004	24.12%	3.450%
28	15.474	2274	2276	2282	rVB2	89156	111084	1.86%	0.267%
29	15.903	2345	2349	2354	rBV	98489	132887	2.23%	0.319%
30	15.974	2356	2361	2374	rBV4	96581	273622	4.59%	0.657%
31	16.403	2430	2434	2436	rBV3	48764	75180	1.26%	0.180%
32	16.439	2437	2440	2446	rVB	93364	148331	2.49%	0.356%

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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-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

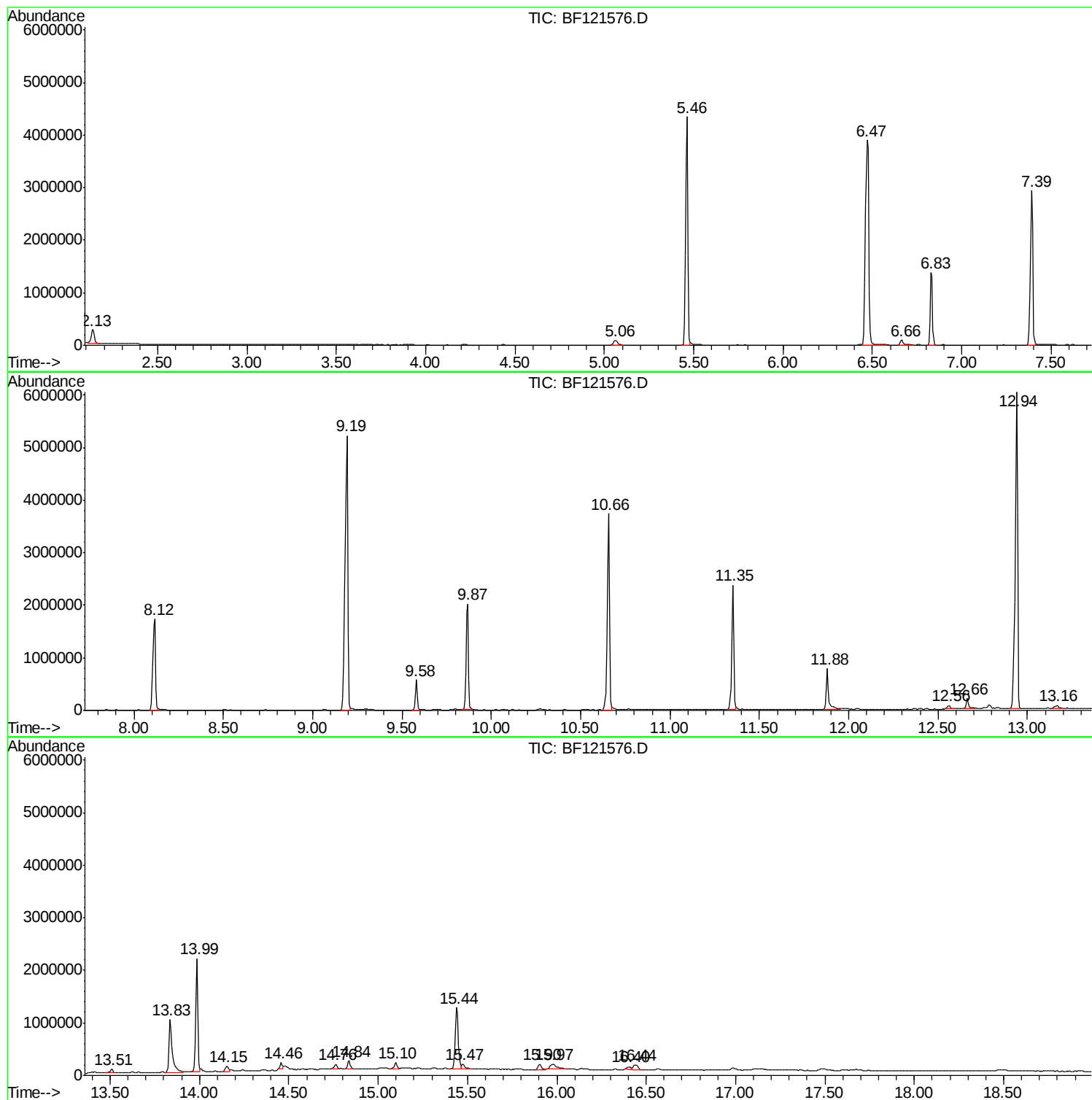
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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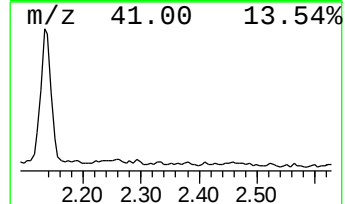
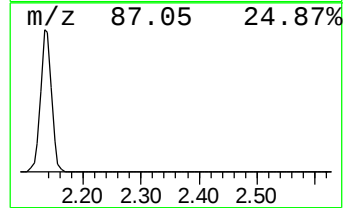
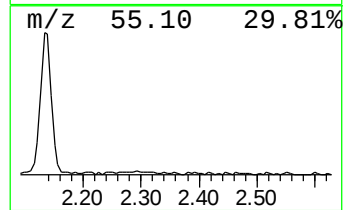
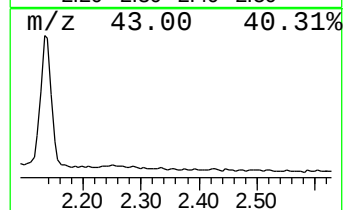
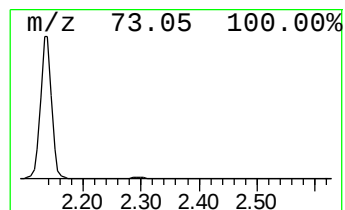
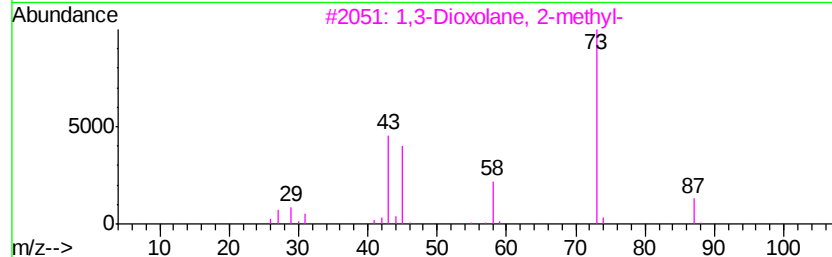
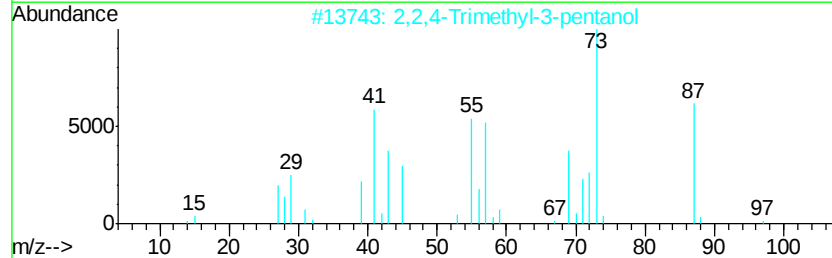
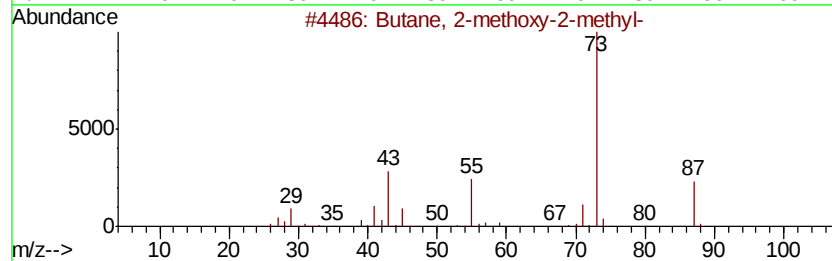
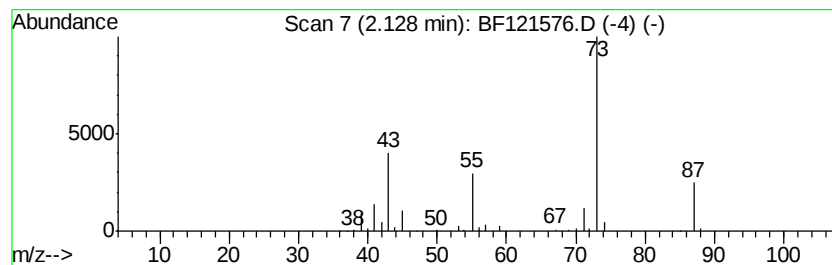
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	5.41 ng	330950	1,4-Dichlorobenzene-d4	6.83

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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12



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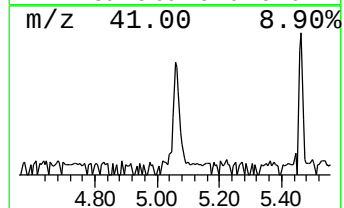
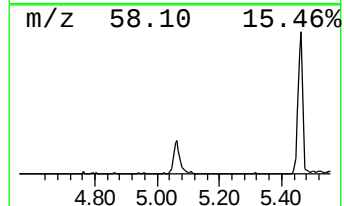
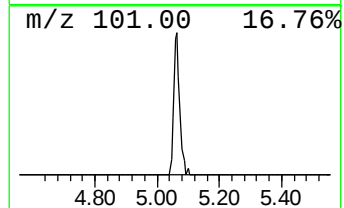
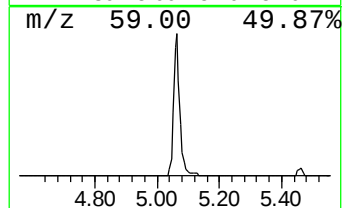
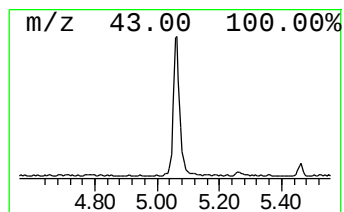
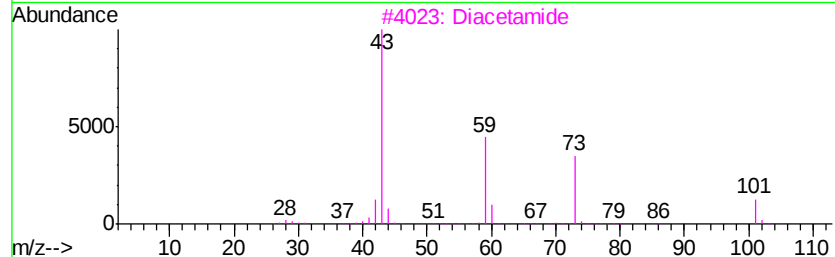
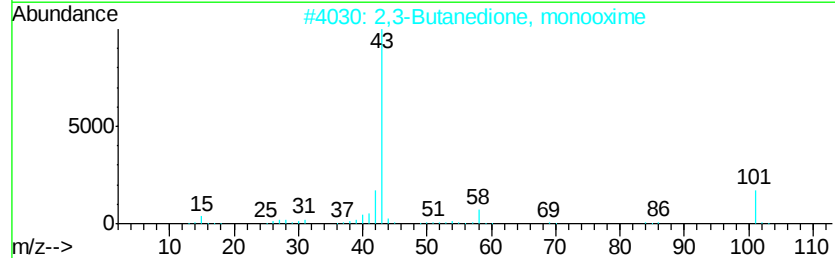
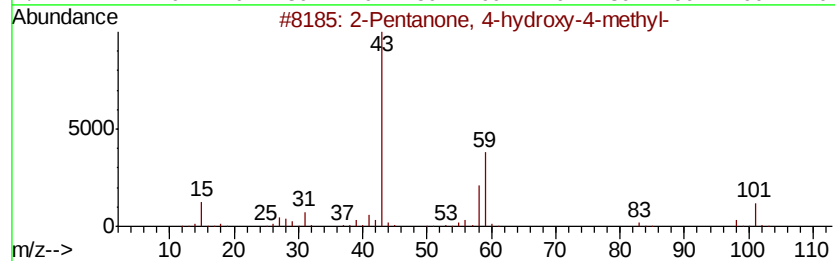
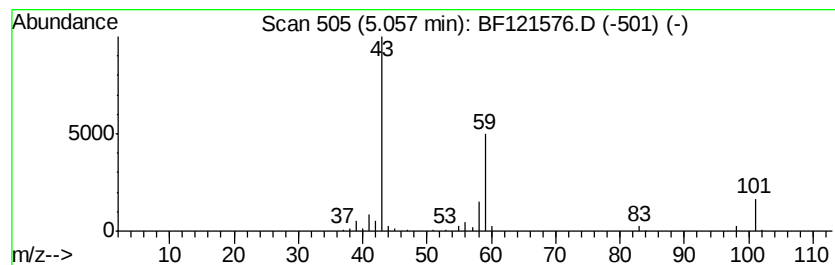
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	2.03 ng	124009	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3			Diacetamide	101	C4H7NO2	000625-77-4	9
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9
5			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9



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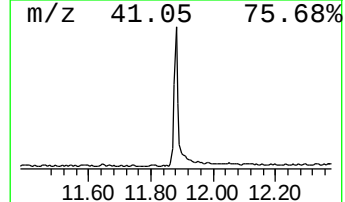
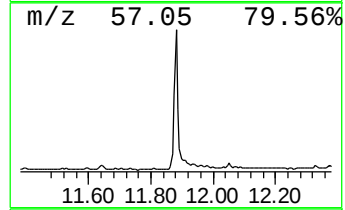
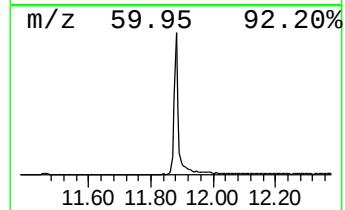
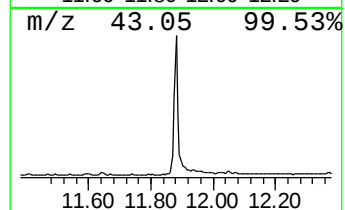
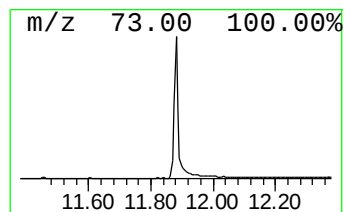
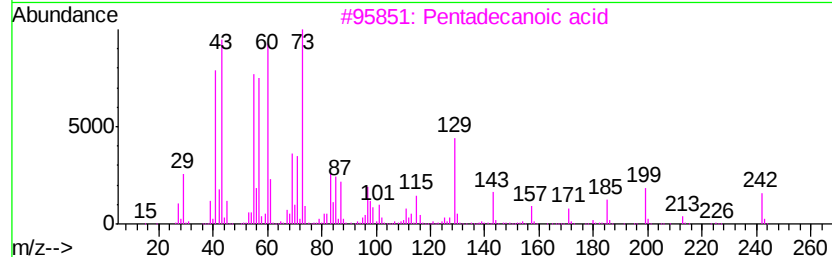
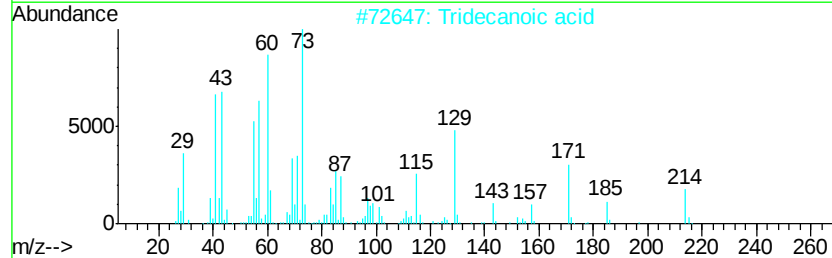
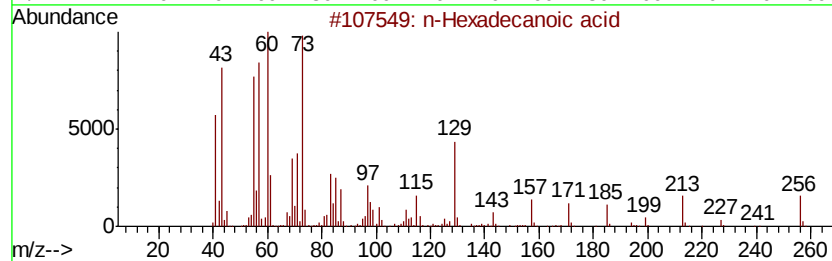
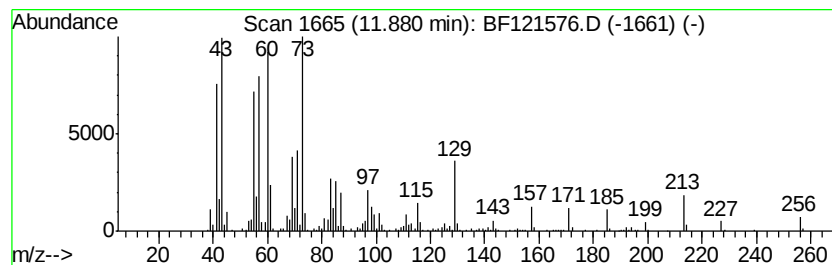
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.88	7.57 ng	770652	Phenanthrene-d10	11.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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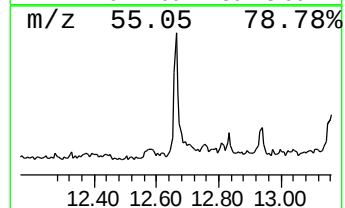
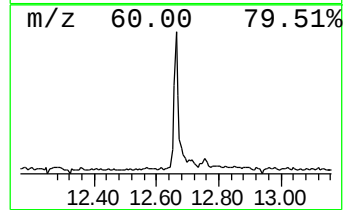
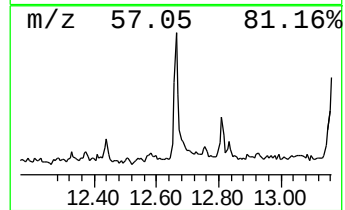
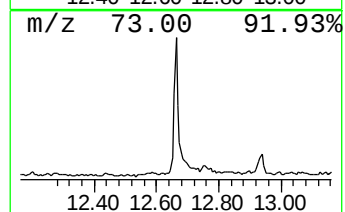
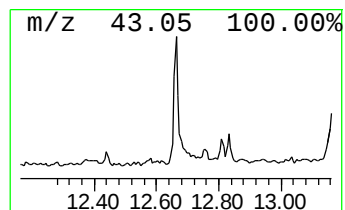
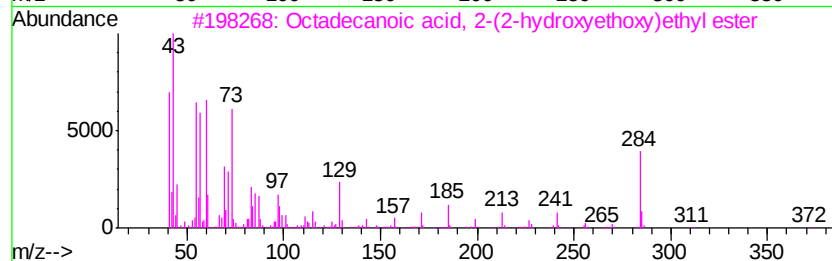
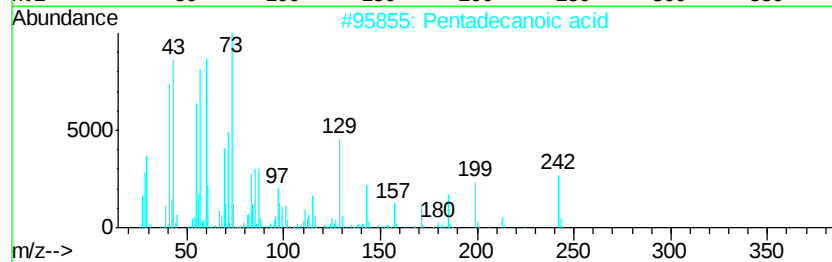
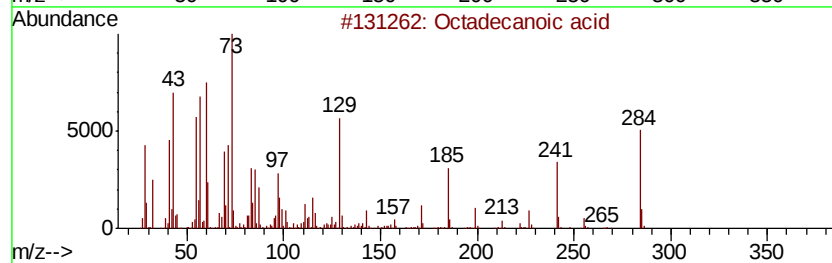
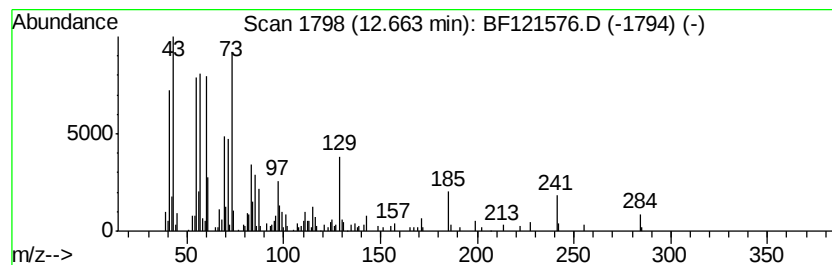
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.66	2.05 ng	208832	Phenanthrene-d10		11.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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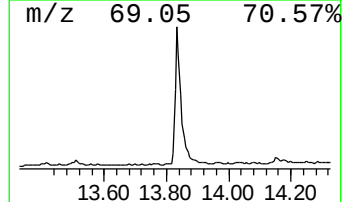
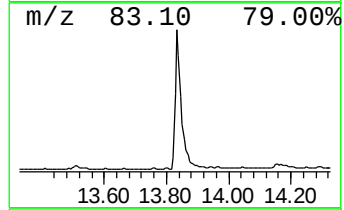
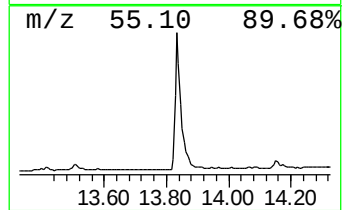
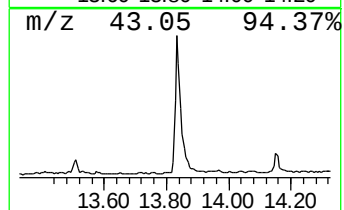
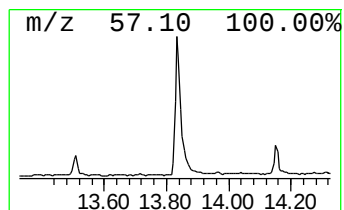
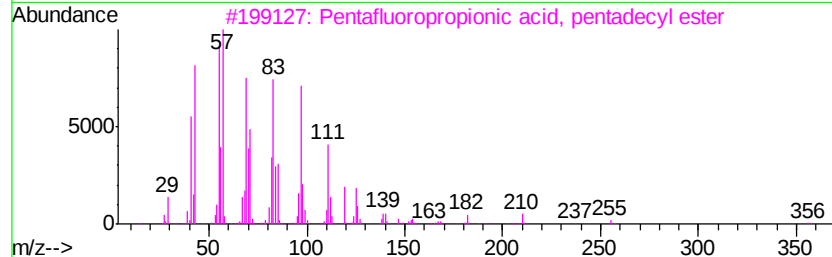
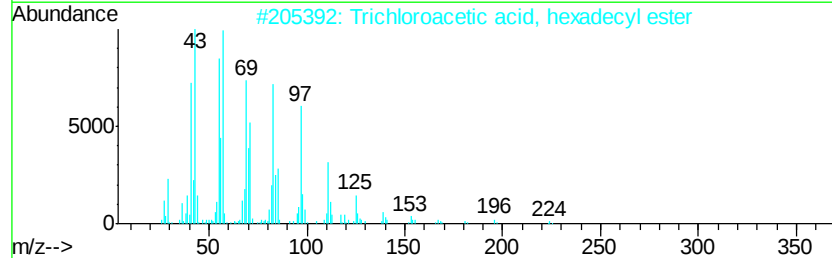
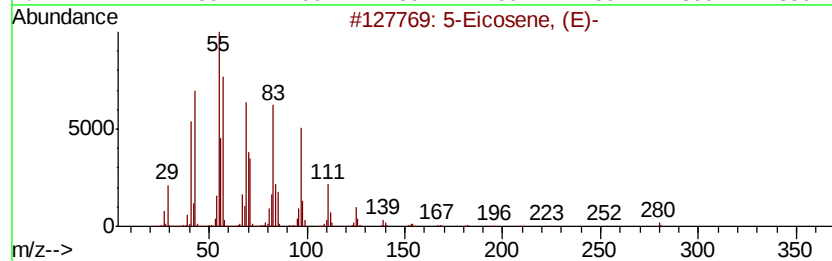
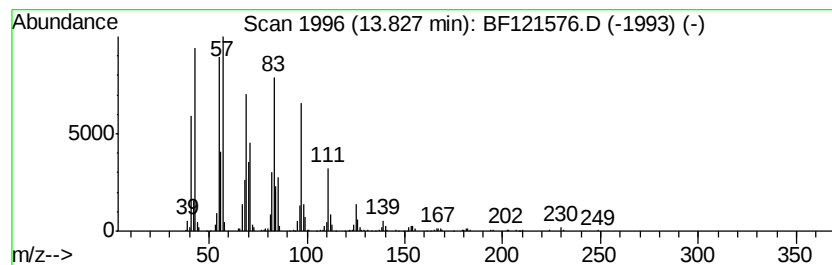
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	14.34 ng	1386180	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4		Cyclopentadecane	210	C15H30	000295-48-7	93
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121576.D
Acq On : 15 Sep 2020 14:27
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-TEST1-ABCD-B

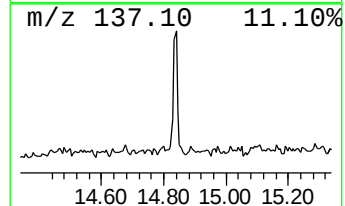
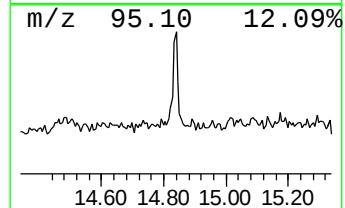
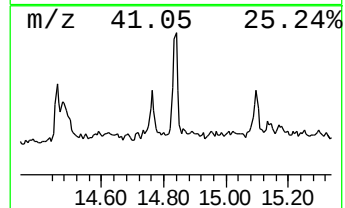
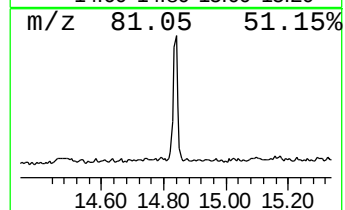
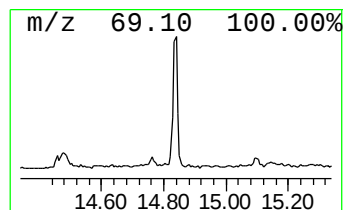
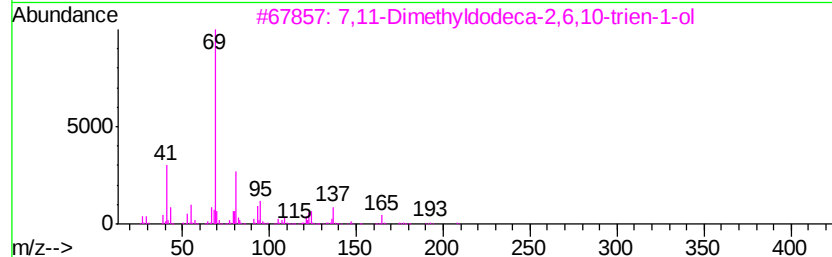
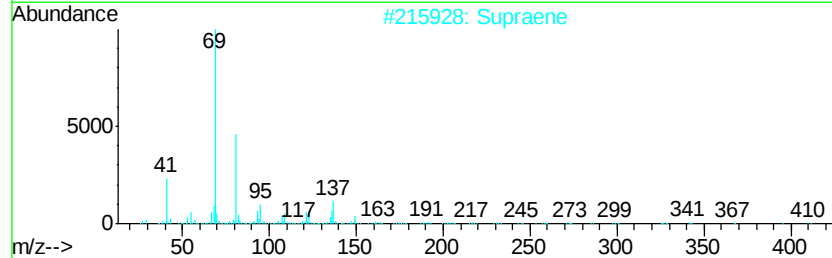
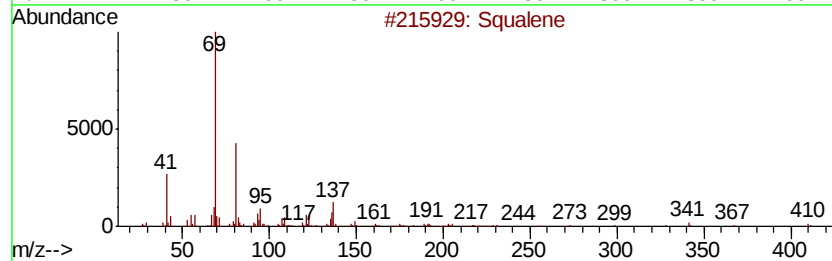
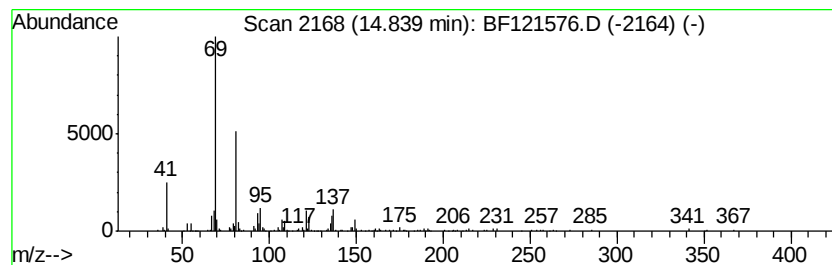
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.26 ng	162381	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Supraene	410	C30H50	007683-64-9	87
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	59
5		Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121576.D
Acq On : 15 Sep 2020 14:27
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-TEST1-ABCD-B

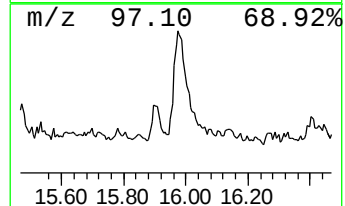
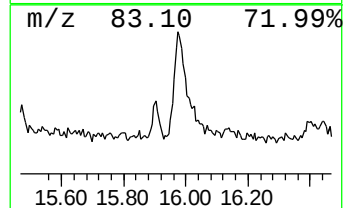
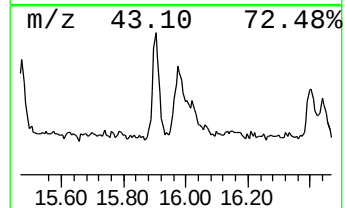
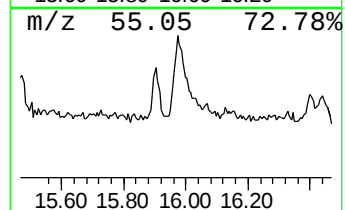
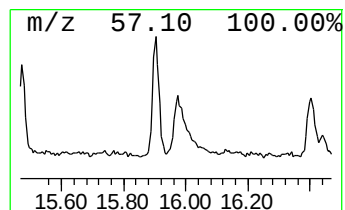
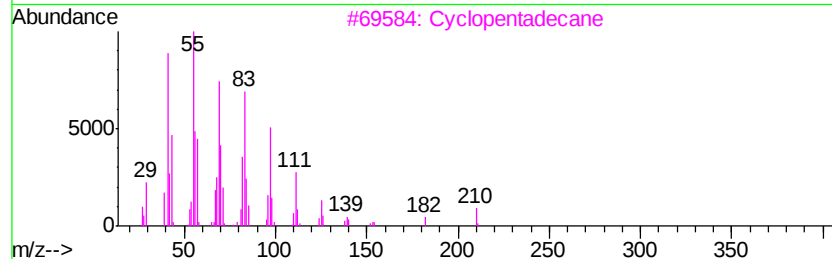
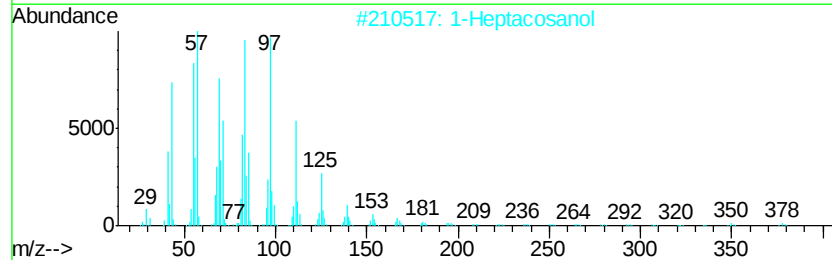
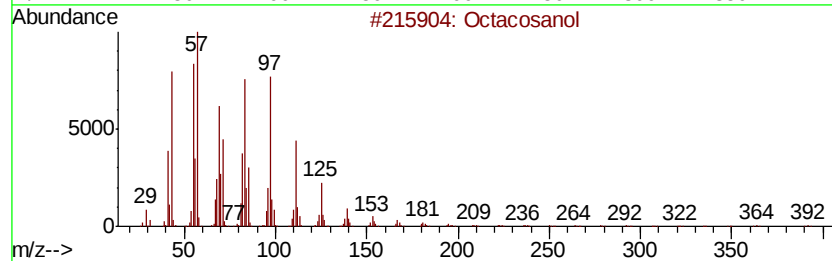
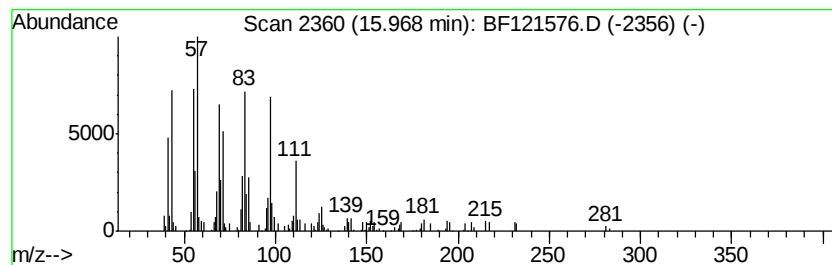
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	3.81 ng	273622	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosanol	410	C28H58O	000557-61-9	93
2		1-Heptacosanol	396	C27H56O	002004-39-9	93
3		Cyclopentadecane	210	C15H30	000295-48-7	93
4		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	93
5		Heptacosyl acetate	438	C29H58O2	1000351-78-2	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121576.D
Acq On : 15 Sep 2020 14:27
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

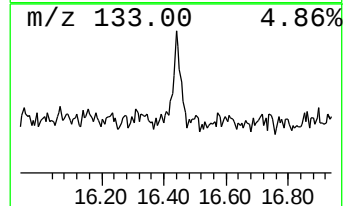
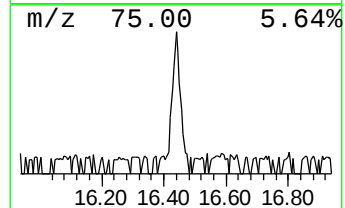
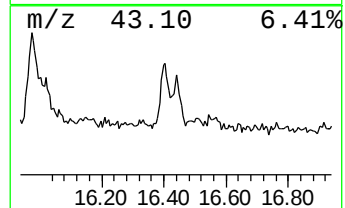
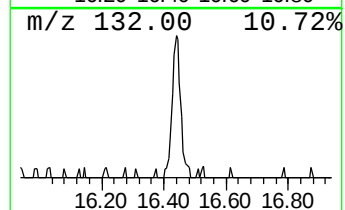
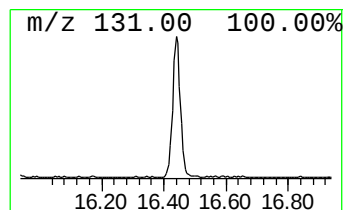
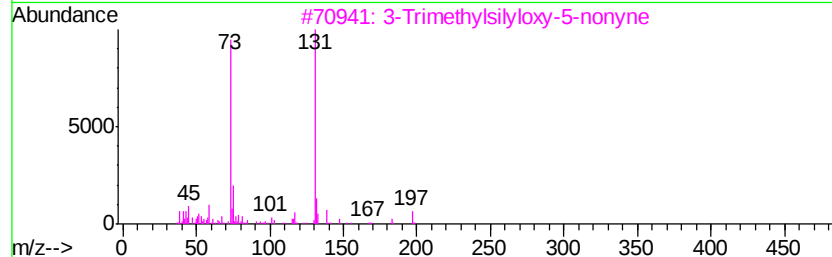
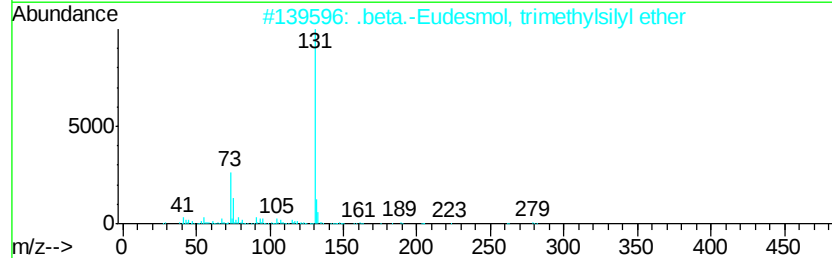
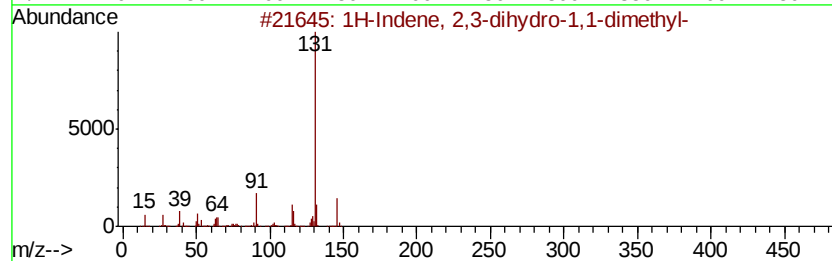
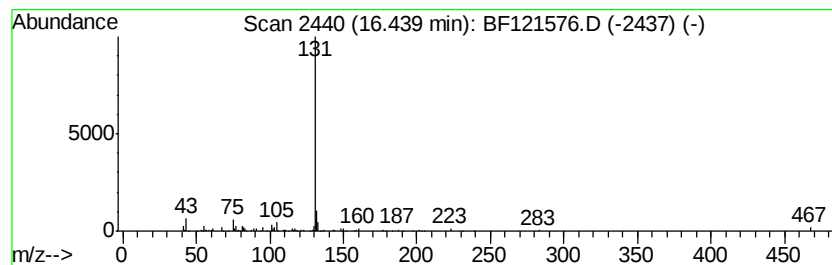
Instrument :
BNA_F
ClientSampleId :
FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1H-Indene, 2,3-dihydro-1,1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.06 ng	148331	Perylene-d12	15.44
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1H-Indene, 2,3-dihydro-1,1-dimet...	146 C11H14	004912-92-9 50
2		.beta.-Eudesmol, trimethylsilyl ...	294 C18H34OSi	1000334-00-1 50
3		3-Trimethylsilyloxy-5-nonyne	212 C12H24OSi	1000245-72-4 43
4		Silane, ethoxytriethyl-	160 C8H20OSi	000597-67-1 40
5		Benzimidazole, 1-(2-chloroethyl)-	180 C9H9ClN2	022492-19-9 38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091520\
Data File : BF121576.D
Acq On : 15 Sep 2020 14:27
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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...	2.13	5.4	ng	330950	1	6.83	1223300	20.0
2-Pentanone, 4-hy...	5.06	2.0	ng	124009	1	6.83	1223300	20.0
n-Hexadecanoic acid	11.88	7.6	ng	770652	4	11.35	2034940	20.0
Octadecanoic acid	12.66	2.0	ng	208832	4	11.35	2034940	20.0
5-Eicosene, (E)-	13.83	14.3	ng	1386180	5	13.99	1932760	20.0
Squalene	14.84	2.3	ng	162381	6	15.44	1437000	20.0
Octacosanol	15.97	3.8	ng	273622	6	15.44	1437000	20.0
1H-Indene, 2,3-di...	16.44	2.1	ng	148331	6	15.44	1437000	20.0