

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101018\
 Data File : BF109743.D
 Acq On : 10 Oct 2018 15:37
 Operator : JU/SJ
 Sample : J5302-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-TW-3-(16.5-17)

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-BF100818.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	4.898	474	478	491	rBV	49612	82800	2.74%	0.350%
2	5.316	545	549	569	rBV	1611996	2033427	67.41%	8.598%
3	6.345	720	724	741	rBV	1763135	2341815	77.63%	9.902%
4	6.469	741	745	768	rVB	2215449	2417077	80.12%	10.221%
5	6.698	780	784	806	rVB	305325	504697	16.73%	2.134%
6	6.851	806	810	831	rBV	1775293	1771880	58.74%	7.492%
7	7.257	875	879	913	rBV	1075744	1561597	51.77%	6.603%
8	7.975	997	1001	1027	rBV	497585	630273	20.89%	2.665%
9	9.051	1180	1184	1210	rBV	2531836	2700899	89.53%	11.421%
10	9.445	1248	1251	1266	rVB	136131	147361	4.88%	0.623%
11	9.722	1294	1298	1318	rBV	776684	766138	25.40%	3.240%
12	10.510	1428	1432	1451	rBV	1629605	1999561	66.28%	8.455%
13	11.198	1546	1549	1560	rBV	679868	844008	27.98%	3.569%
14	11.739	1638	1641	1656	rBV2	72414	104433	3.46%	0.442%
15	12.786	1814	1819	1837	rBV	2667910	3016704	100.00%	12.756%
16	13.680	1967	1971	1983	rBV2	140852	248775	8.25%	1.052%
17	13.827	1992	1996	2010	rBV	838579	945048	31.33%	3.996%
18	13.998	2021	2025	2032	rBV	31721	32601	1.08%	0.138%
19	14.304	2071	2077	2087	rBV	43984	62639	2.08%	0.265%
20	14.592	2123	2126	2132	rVB	52721	53650	1.78%	0.227%
21	14.662	2134	2138	2145	rVV	236023	216150	7.17%	0.914%
22	14.904	2175	2179	2184	rBV	65237	70781	2.35%	0.299%
23	15.227	2229	2234	2250	rBV	592219	918113	30.43%	3.882%
24	15.645	2301	2305	2311	rBV	54064	76792	2.55%	0.325%
25	15.709	2311	2316	2322	rBV7	17116	43217	1.43%	0.183%
26	16.103	2377	2383	2388	rBV	34116	58394	1.94%	0.247%

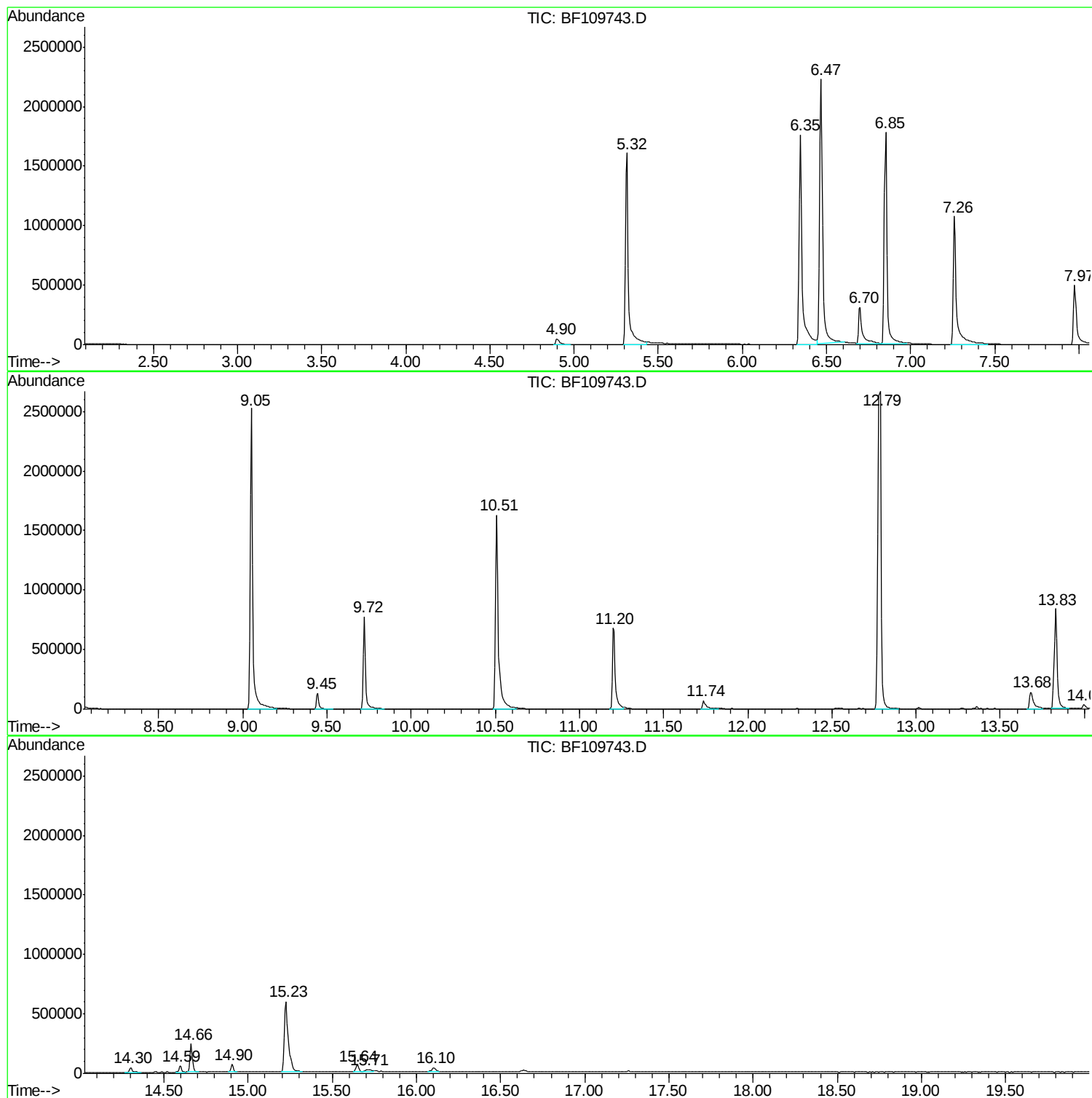
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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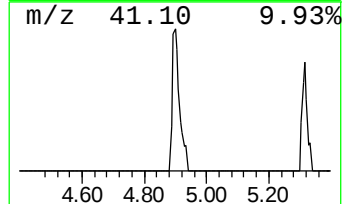
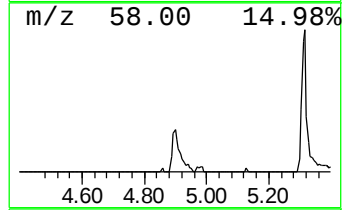
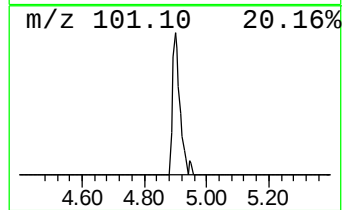
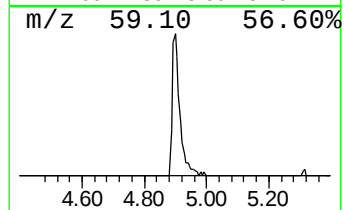
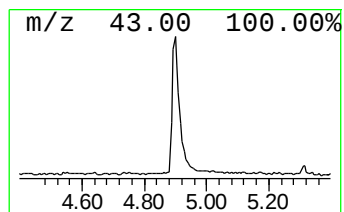
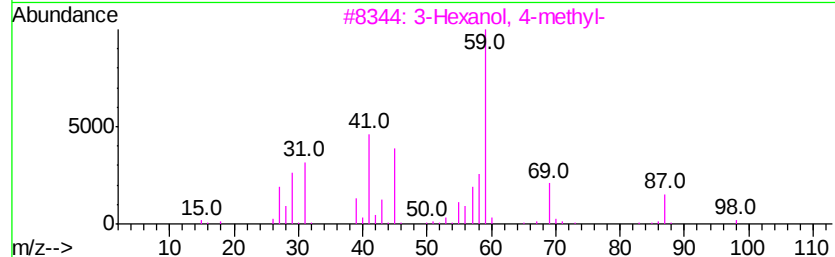
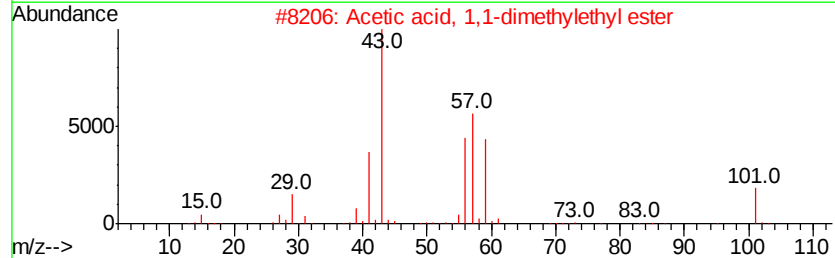
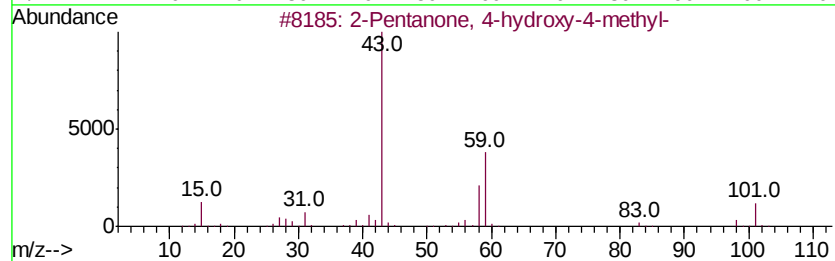
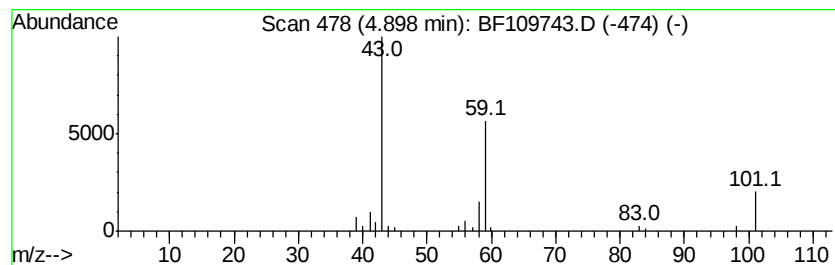
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.28 ng	82800	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5			2-Propenoic acid, 3-methoxybutyl...	158	C8H14O3	002768-07-2	9



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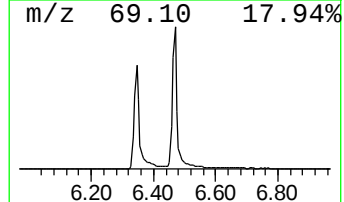
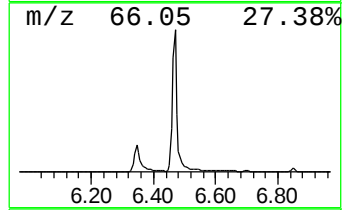
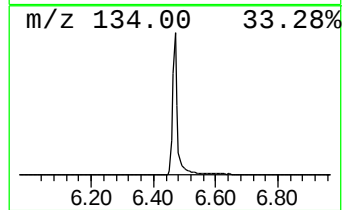
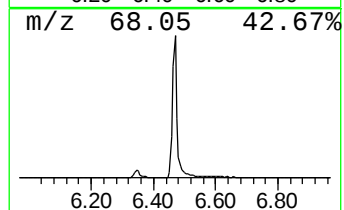
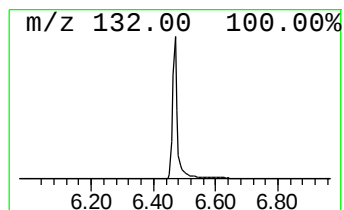
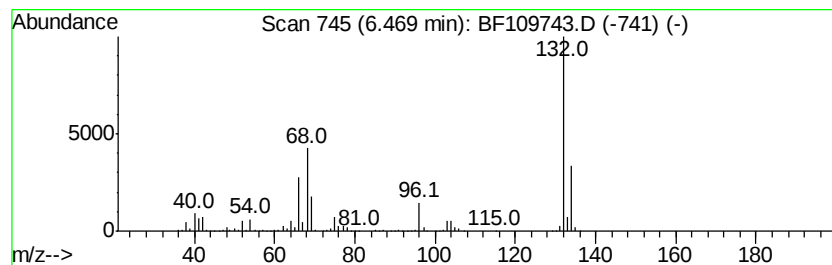
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	95.78 ng	2417080	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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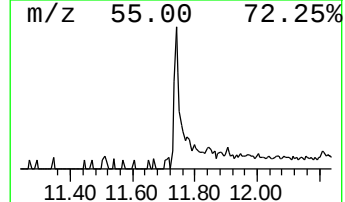
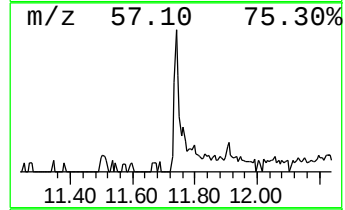
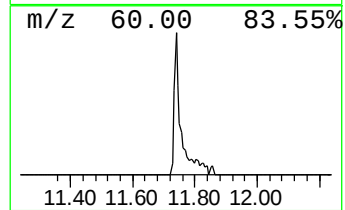
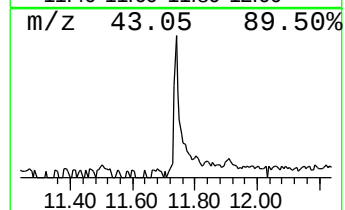
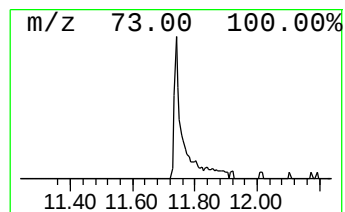
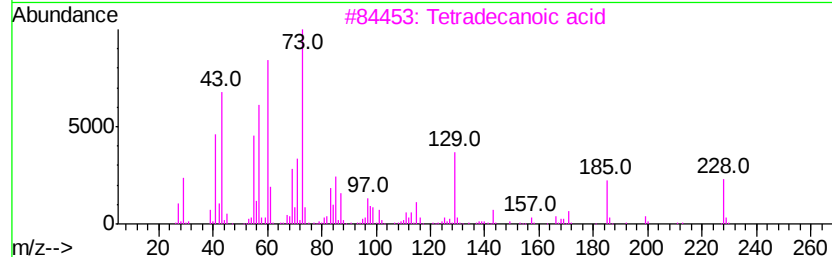
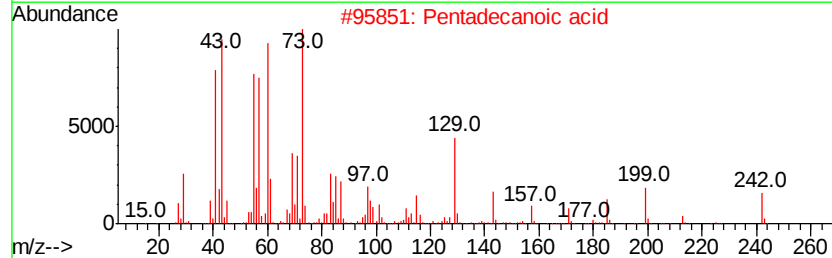
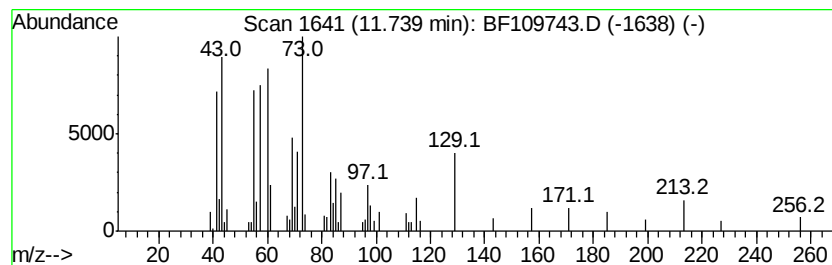
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 Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.47 ng	104433	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	15
5		Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	11



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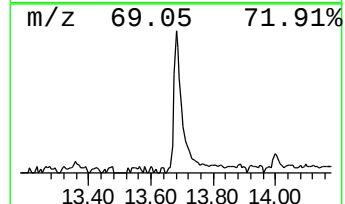
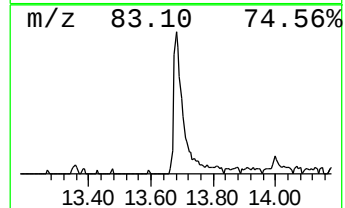
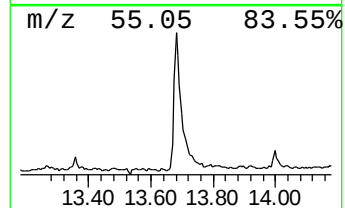
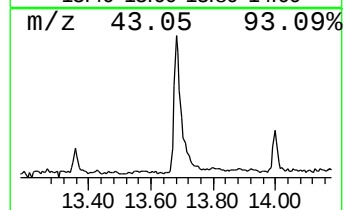
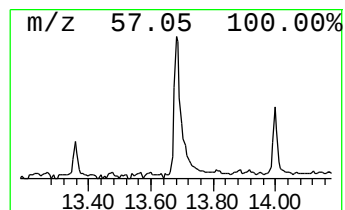
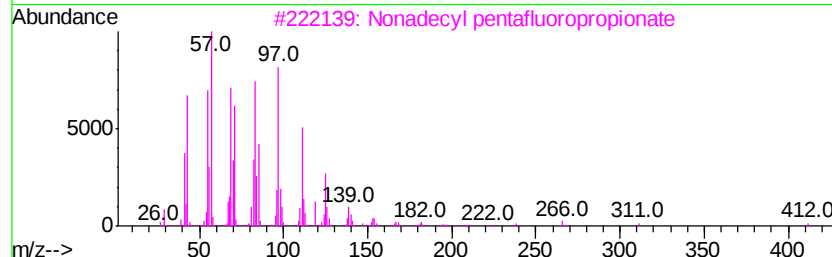
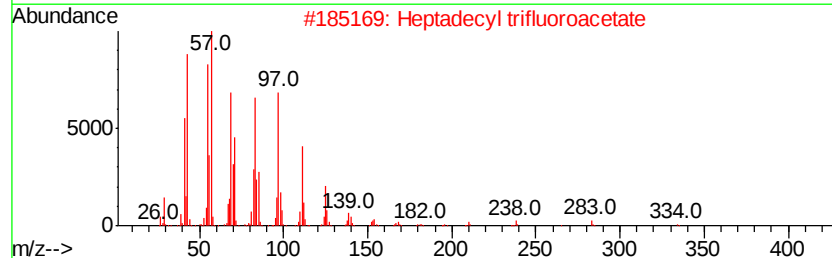
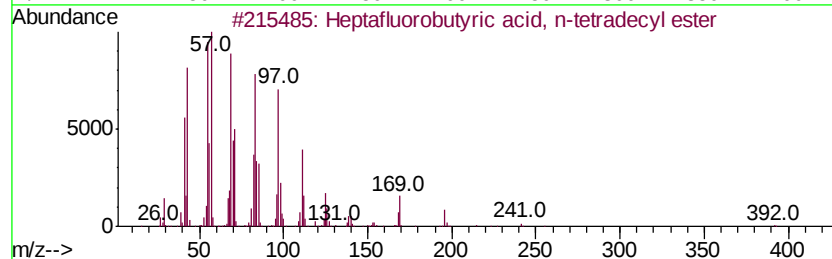
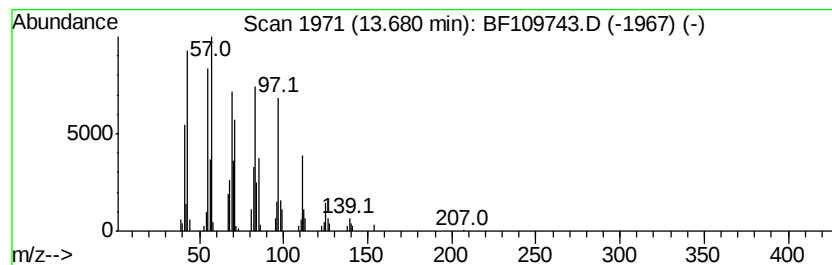
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.68	5.26 ng	248775	Chrysene-d12	13.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4		1-Docosene	308	C22H44	001599-67-3	91
5		1-Heptacosanol	396	C27H56O	002004-39-9	91



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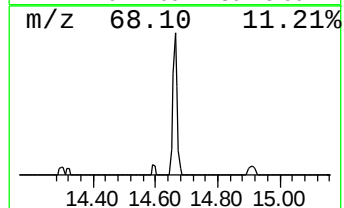
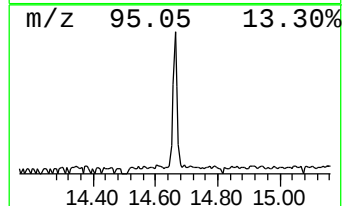
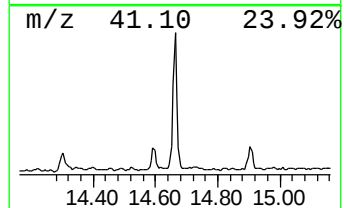
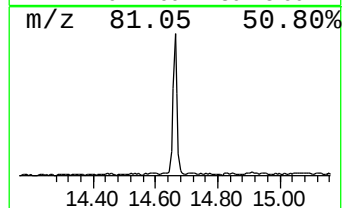
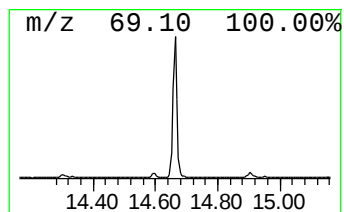
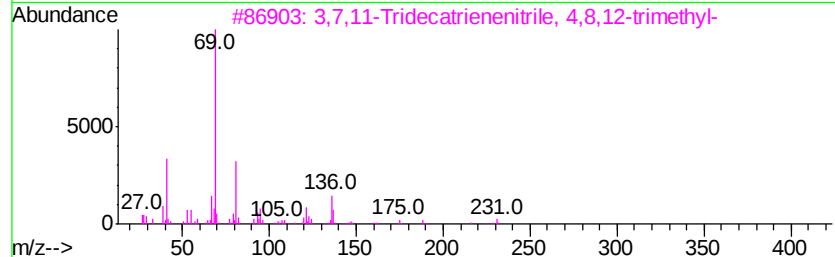
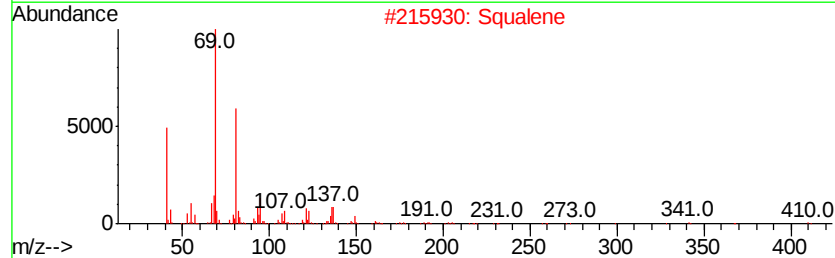
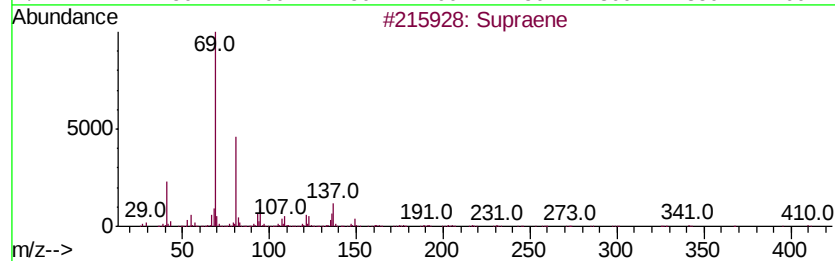
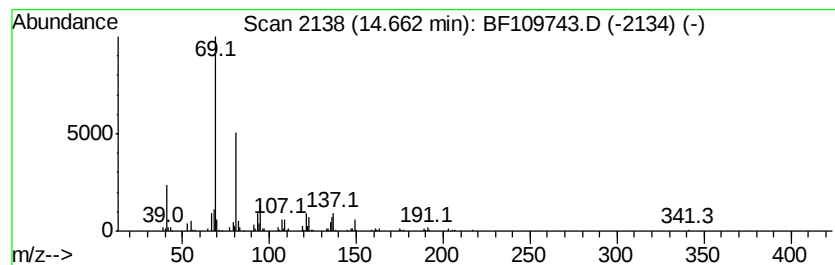
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	4.71 ng	216150	Perylene-d12	15.23

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		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	3.3	ng	82800	1	6.70	504697	20.0
unknown6.47	6.47	95.8	ng	2417080	1	6.70	504697	20.0
n-Hexadecanoic acid	11.74	2.5	ng	104433	4	11.20	844008	20.0
Heptafluorobutyri...	13.68	5.3	ng	248775	5	13.83	945048	20.0
Supraene	14.66	4.7	ng	216150	6	15.23	918113	20.0