

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102822\
 Data File : BG055357.D
 Acq On : 29 Oct 2022 1:31
 Operator : CG/JU
 Sample : N5235-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LSP-GW-03-DUP

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_G\Methods\8270-BG102422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055357.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.303	337	343	353	rBV	335553	500387	19.34%	4.604%
2	5.785	419	425	439	rVB	238360	383591	14.82%	3.529%
3	7.407	694	701	709	rBV	140221	247008	9.55%	2.273%
4	8.259	840	846	852	rBV	108351	178327	6.89%	1.641%
5	9.434	1038	1046	1057	rBV	353177	646738	24.99%	5.950%
6	11.091	1320	1328	1334	rBV	151314	271222	10.48%	2.495%
7	11.144	1334	1337	1344	rVB	20688	31240	1.21%	0.287%
8	12.730	1600	1607	1613	rVB	19180	31023	1.20%	0.285%
9	12.942	1633	1643	1650	rVB	23914	38913	1.50%	0.358%
10	13.500	1731	1738	1746	rBV	1051842	1630992	63.03%	15.006%
11	14.875	1963	1972	1978	rBV	271062	411835	15.92%	3.789%
12	14.939	1978	1983	1989	rVB	28628	42462	1.64%	0.391%
13	15.268	2031	2039	2048	rBV	22821	35896	1.39%	0.330%
14	15.915	2142	2149	2159	rVB	30784	47833	1.85%	0.440%
15	16.355	2217	2224	2234	rBV	763665	1196171	46.23%	11.005%
16	17.607	2430	2437	2442	rBV	354021	523045	20.21%	4.812%
17	17.648	2442	2444	2451	rVB	41385	49636	1.92%	0.457%
18	18.006	2497	2505	2511	rBV	32307	48188	1.86%	0.443%
19	18.247	2539	2546	2550	rBV4	16761	27431	1.06%	0.252%
20	18.459	2578	2582	2590	rBV5	41799	74976	2.90%	0.690%
21	19.716	2791	2796	2805	rBV7	13276	30245	1.17%	0.278%
22	20.180	2869	2875	2881	rBV	1991693	2587593	100.00%	23.807%
23	20.456	2917	2922	2930	rBV3	18334	29868	1.15%	0.275%
24	20.950	3002	3006	3010	rBV2	32003	39077	1.51%	0.360%
25	21.479	3090	3096	3115	rBV2	115712	353387	13.66%	3.251%
26	21.878	3158	3164	3174	rBV	335191	583390	22.55%	5.367%
27	22.031	3186	3190	3196	rBV	25290	35782	1.38%	0.329%
28	22.665	3293	3298	3303	rBV	22082	37158	1.44%	0.342%
29	23.388	3416	3421	3428	rVB2	20216	40156	1.55%	0.369%
30	23.594	3450	3456	3465	rVB	39182	76514	2.96%	0.704%
31	24.234	3561	3565	3574	rVB4	17061	33547	1.30%	0.309%
32	25.268	3730	3741	3752	rVB2	196804	605404	23.40%	5.570%

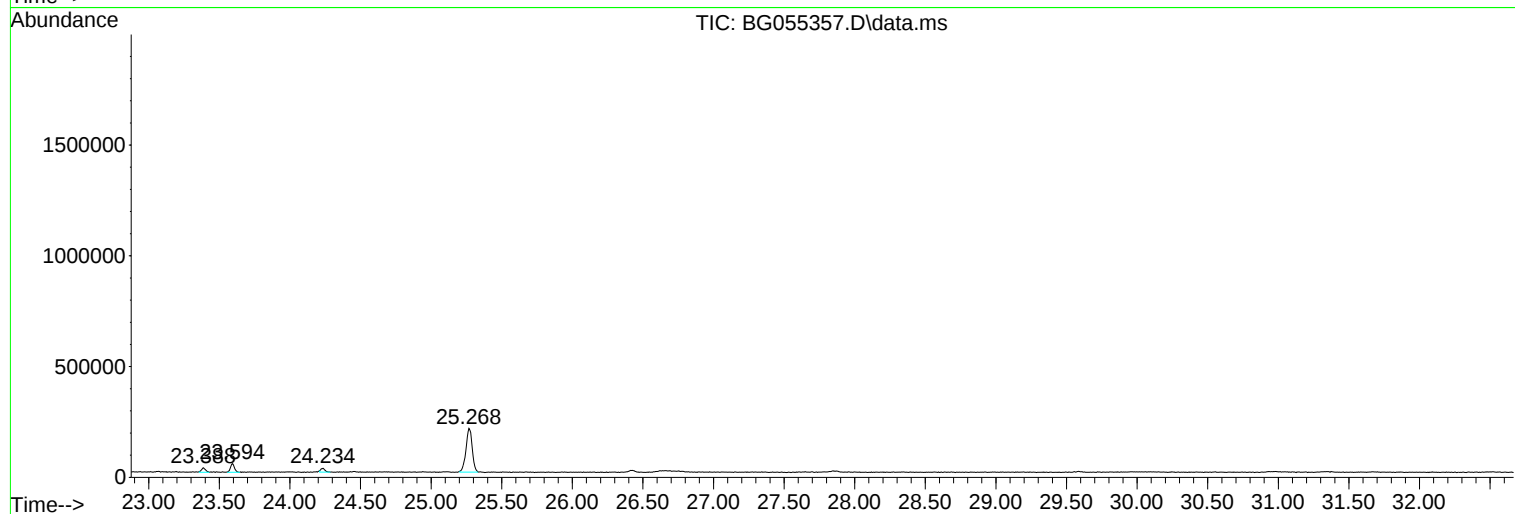
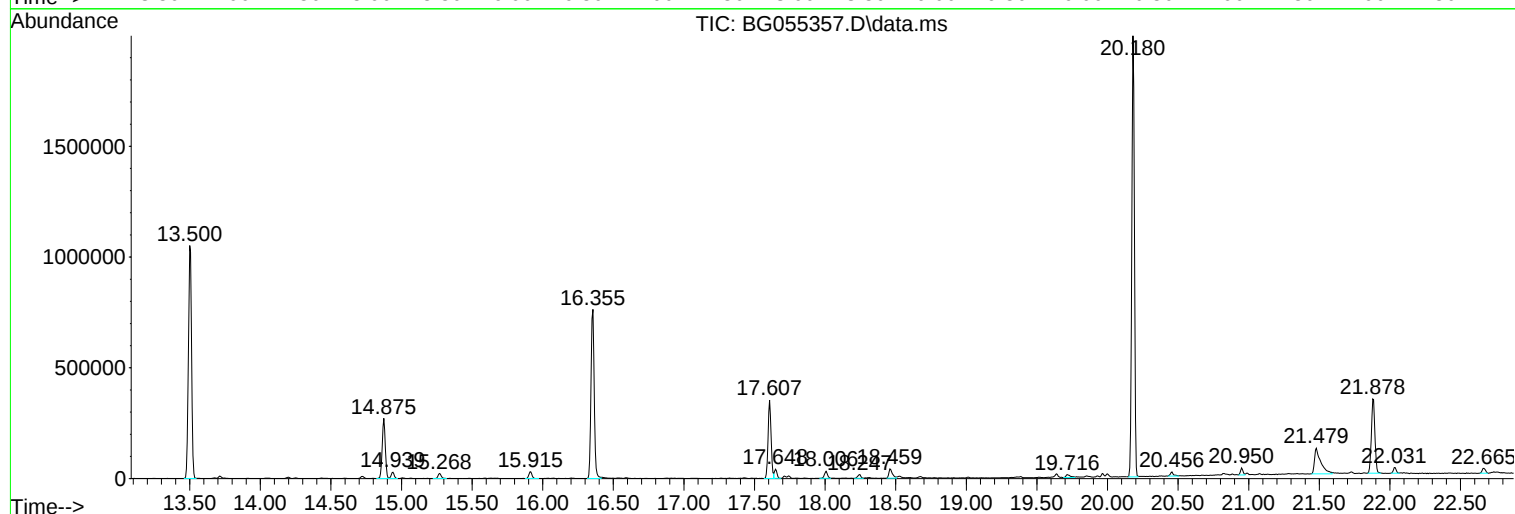
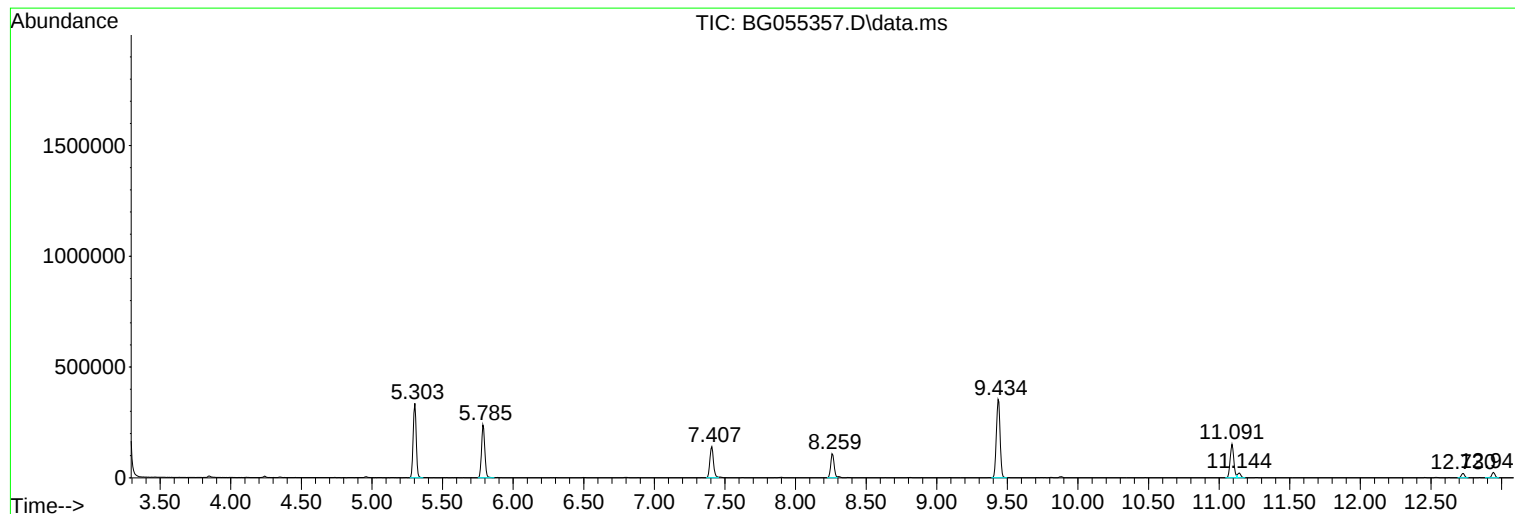
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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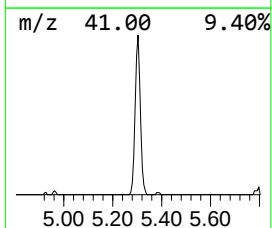
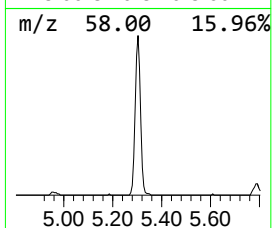
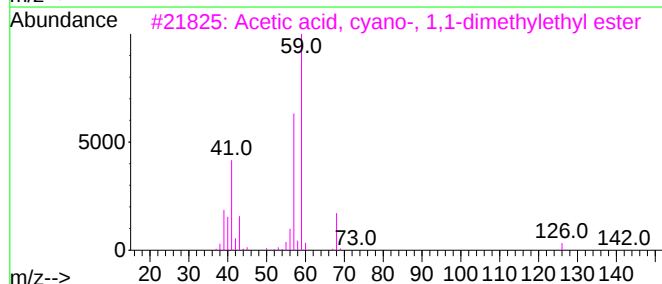
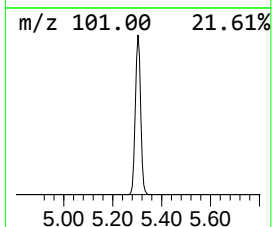
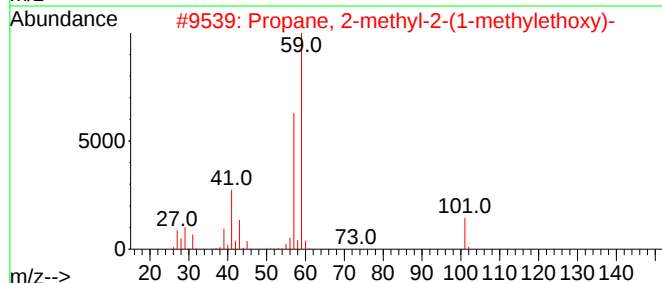
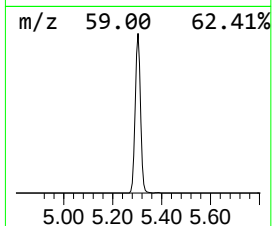
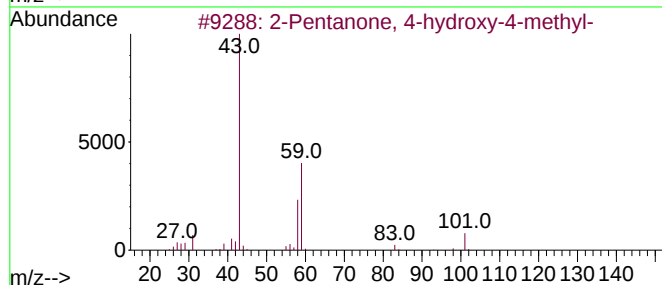
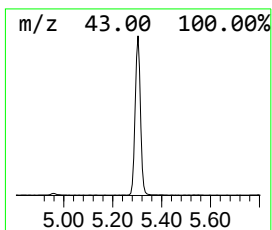
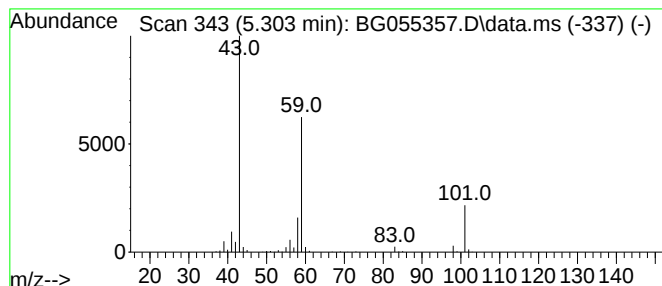
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.303	56.12 ng	500387	1,4-Dichlorobenzene-d4	8.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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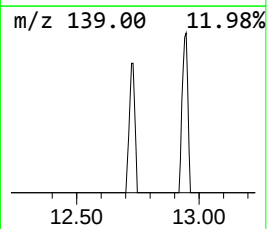
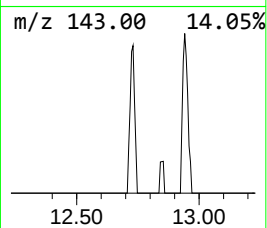
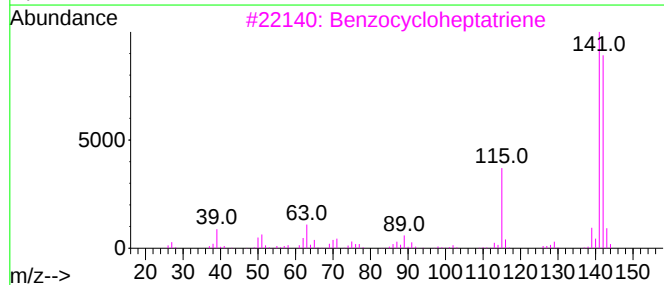
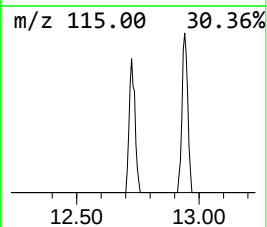
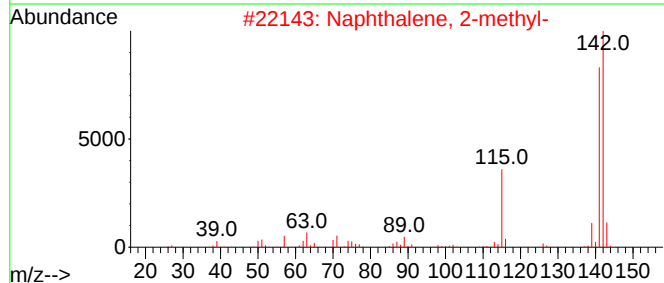
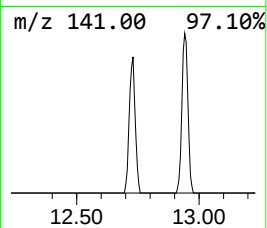
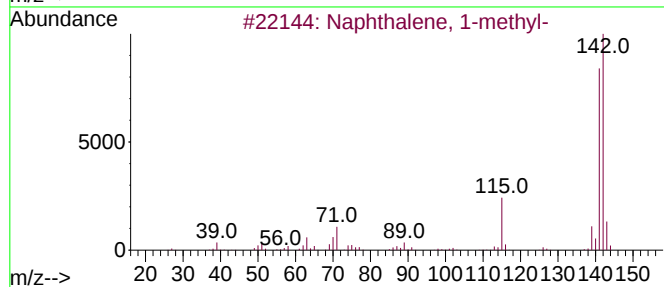
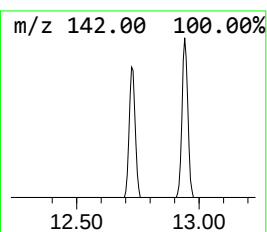
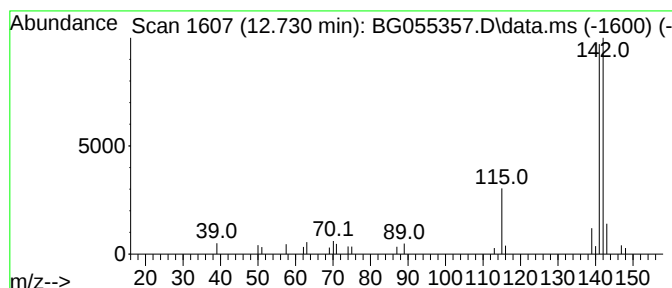
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.730	2.29 ng	31023	Naphthalene-d8	11.091

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	64



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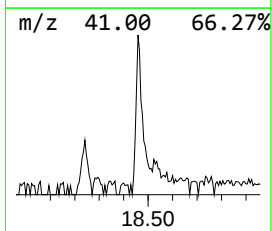
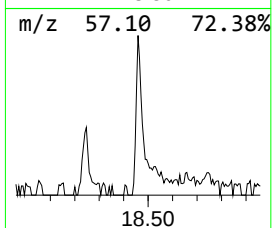
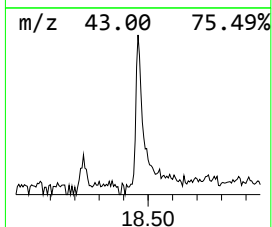
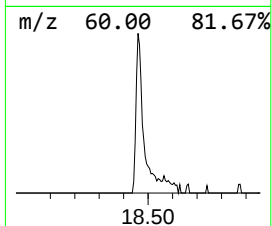
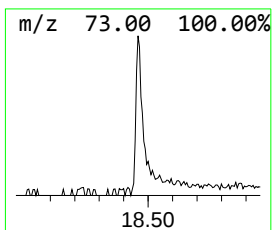
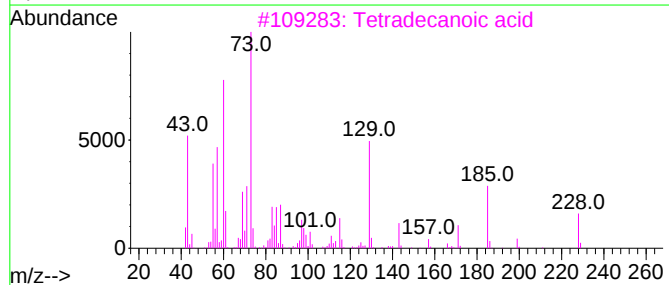
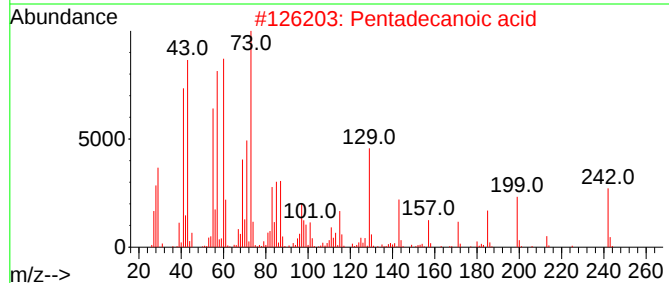
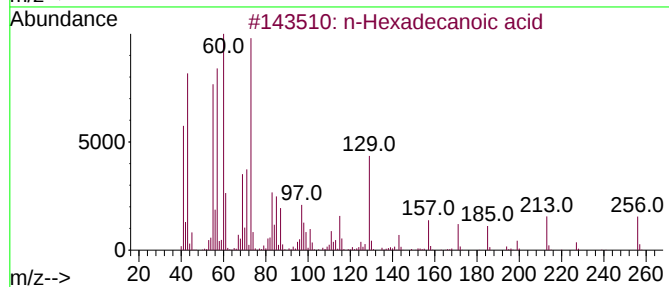
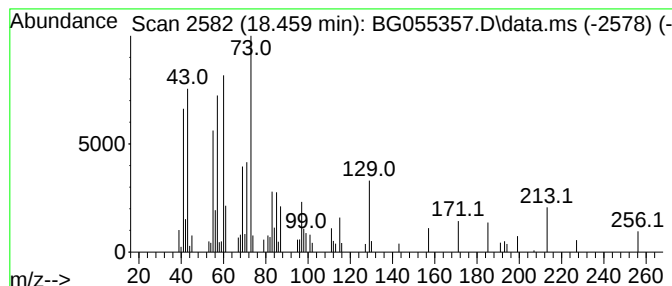
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.459	2.87 ng	74976	Phenanthrene-d10	17.607

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25
5			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20



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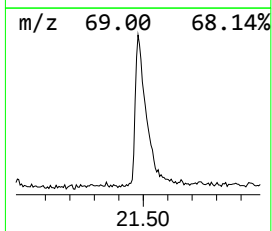
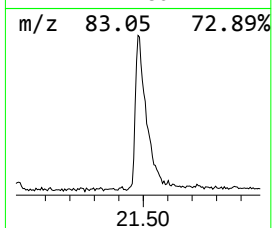
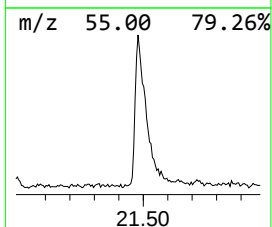
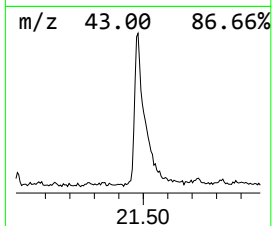
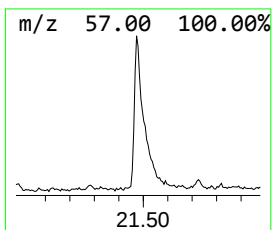
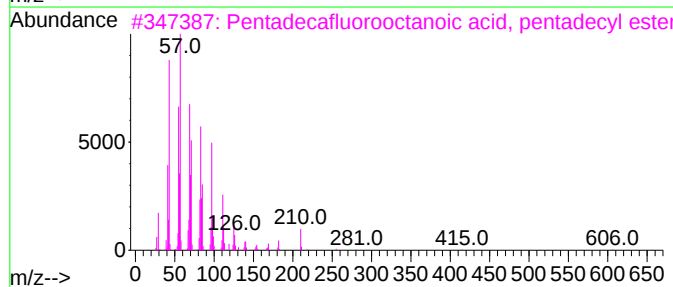
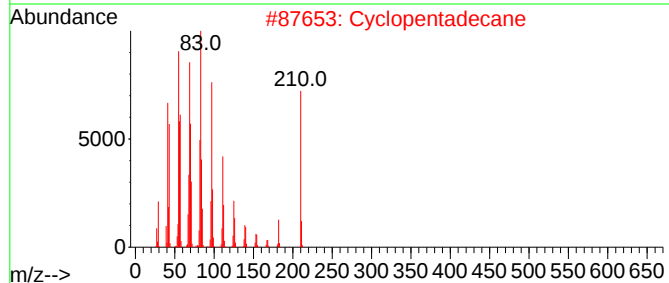
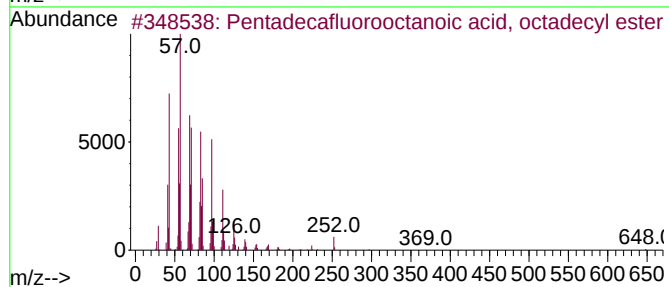
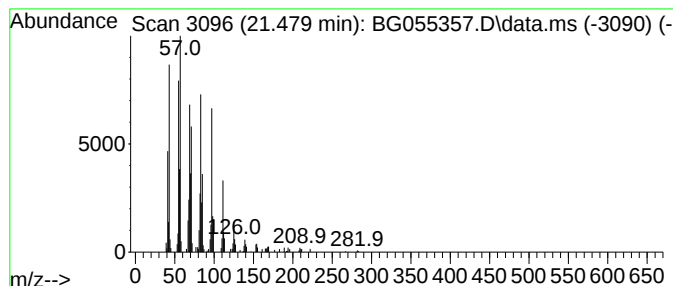
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.479	12.11 ng	353387	Chrysene-d12	21.878	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Cyclopentadecane	210	C15H30	000295-48-7	94
3	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93



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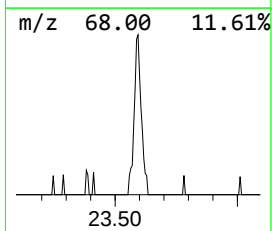
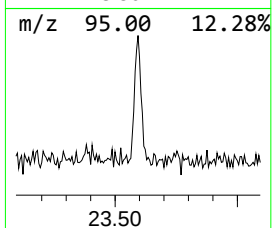
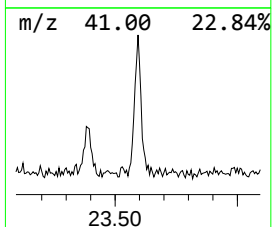
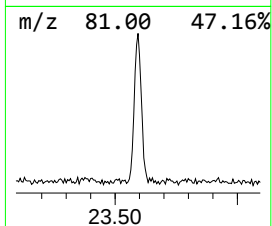
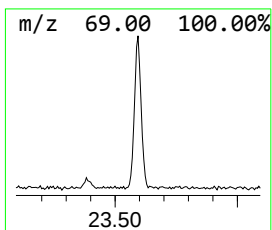
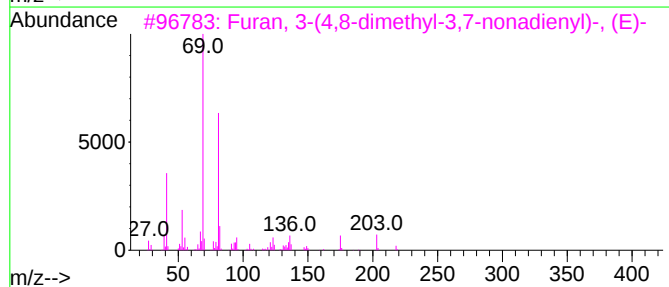
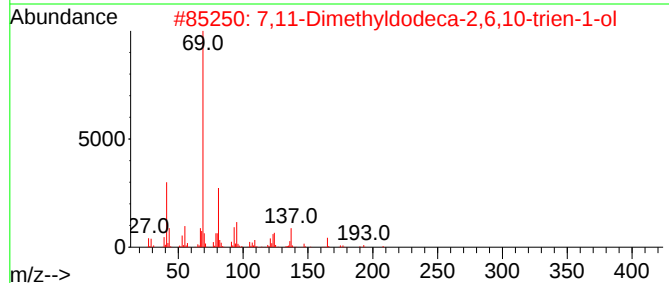
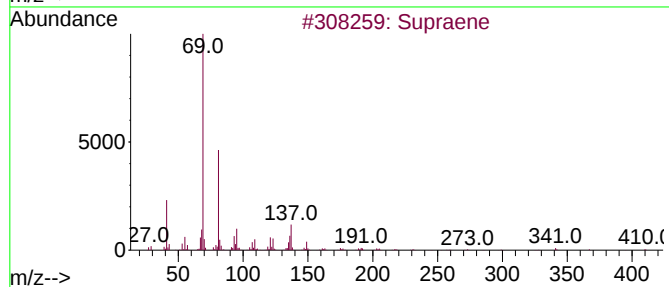
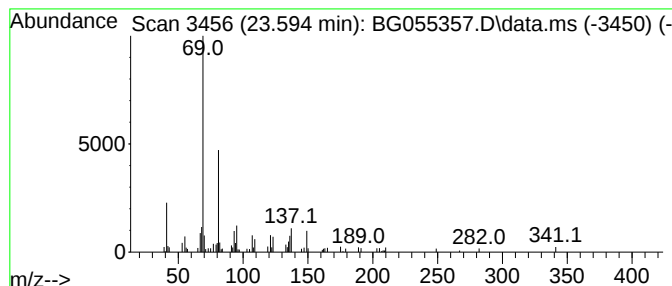
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Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.594	2.53 ng	76514	Perylene-d12	25.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	68
3			Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	64
4			Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	59
5			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	53



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.303	56.1	ng	500387	1	8.259	178327	20.0
Benzocyclohepta...	12.730	2.3	ng	31023	2	11.091	271222	20.0
n-Hexadecanoic ...	18.459	2.9	ng	74976	4	17.607	523045	20.0
Pentadecafluoro...	21.479	12.1	ng	353387	5	21.878	583390	20.0
Supraene	23.594	2.5	ng	76514	6	25.268	605404	20.0