

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121421\
 Data File : BP008407.D
 Acq On : 14 Dec 2021 23:02
 Operator : CG/JU
 Sample : M5076-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-11-G

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_P\Methods\8270E-BP121421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	316	321	334	rVB	313875	442311	25.02%	3.809%
2	5.346	395	401	423	rVB	739722	1171336	66.27%	10.086%
3	5.946	498	503	508	rBV	23968	33124	1.87%	0.285%
4	6.940	665	672	699	rBV	690911	1254545	70.97%	10.803%
5	7.746	802	809	817	rBV	201133	328333	18.57%	2.827%
6	8.910	998	1007	1023	rBV	435241	798939	45.20%	6.880%
7	10.540	1276	1284	1296	rBV	229359	423456	23.96%	3.646%
8	13.016	1697	1705	1727	rBV	1046136	1605546	90.83%	13.825%
9	14.063	1876	1883	1889	rBV3	9836	21062	1.19%	0.181%
10	14.398	1932	1940	1952	rBV	334328	525158	29.71%	4.522%
11	15.898	2186	2195	2214	rBV	606961	1042247	58.96%	8.975%
12	17.087	2392	2397	2403	rVB3	18032	23392	1.32%	0.201%
13	17.163	2403	2410	2421	rBV	318853	538813	30.48%	4.640%
14	18.069	2560	2564	2568	rBV6	12331	20565	1.16%	0.177%
15	19.733	2841	2847	2858	rBV	1390495	1767645	100.00%	15.221%
16	20.975	3055	3058	3066	rBV5	52494	80043	4.53%	0.689%
17	21.269	3103	3108	3119	rBV	444452	652109	36.89%	5.615%
18	22.492	3312	3316	3322	rVB	114454	168910	9.56%	1.454%
19	23.633	3504	3510	3524	rVB2	333981	715724	40.49%	6.163%

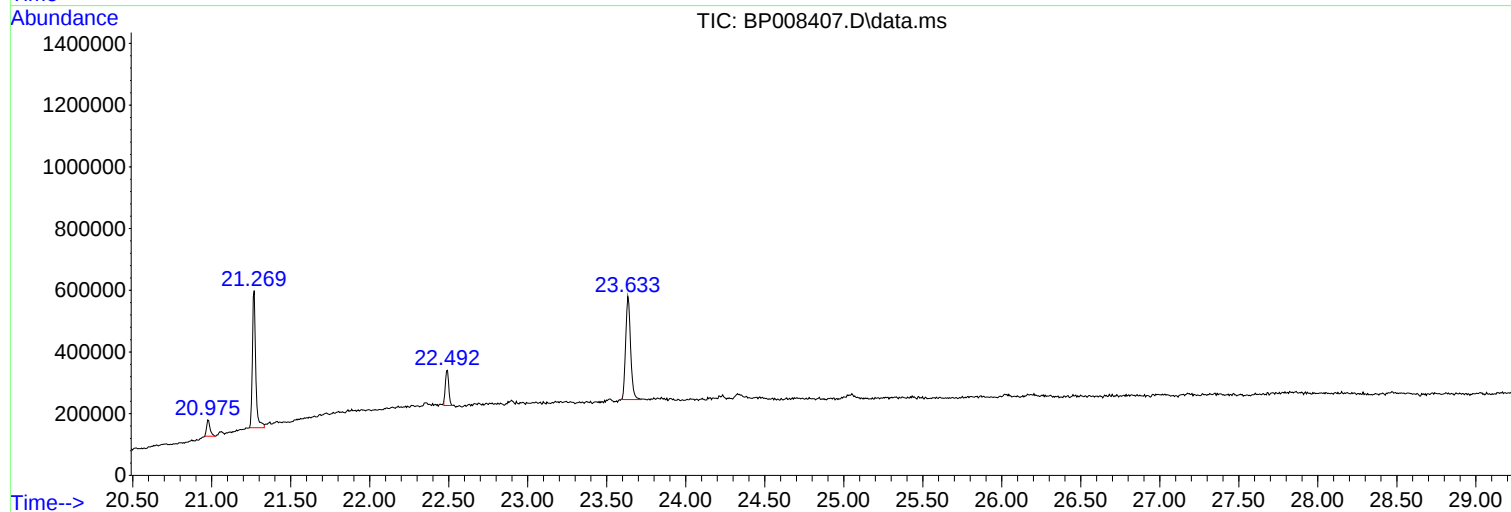
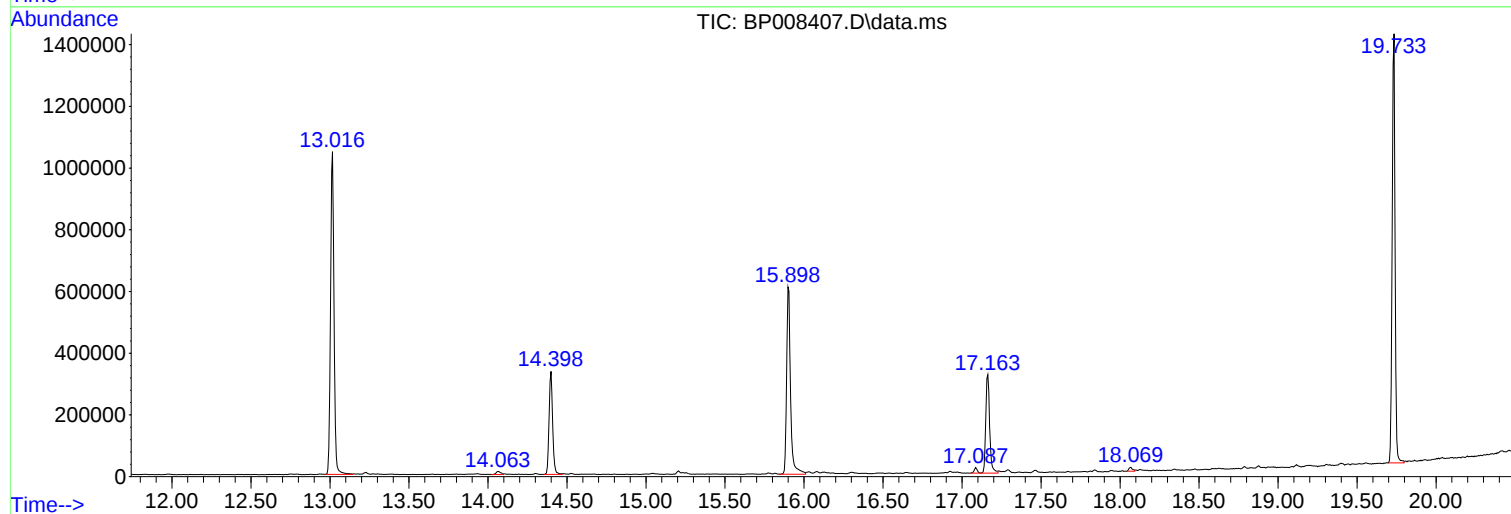
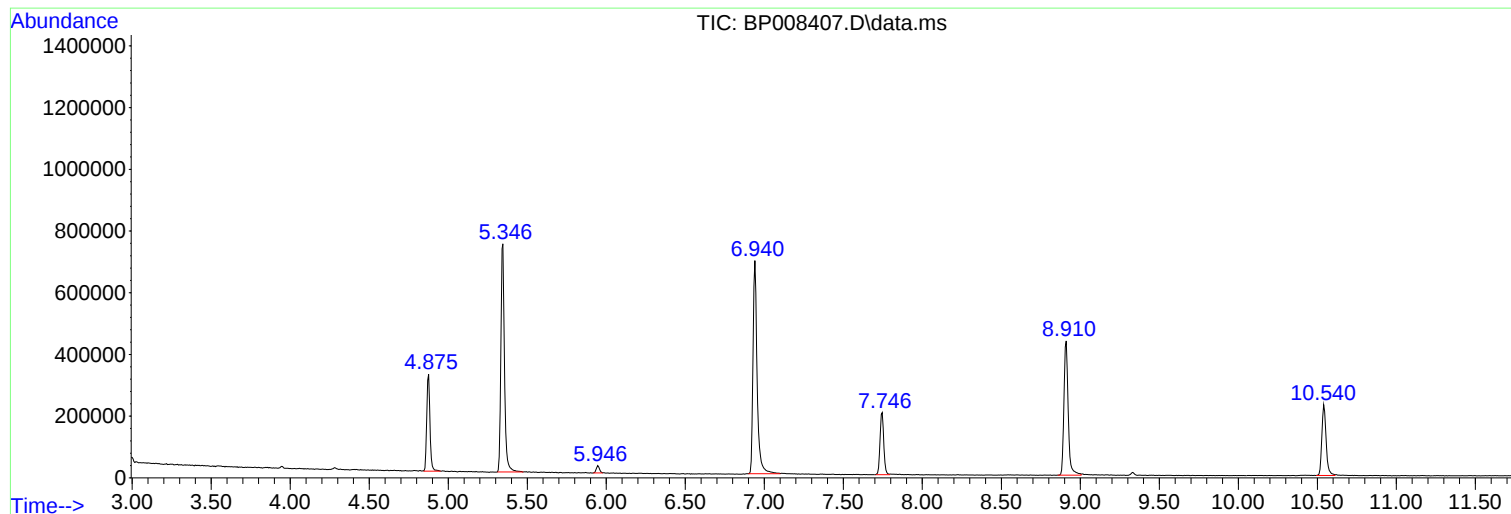
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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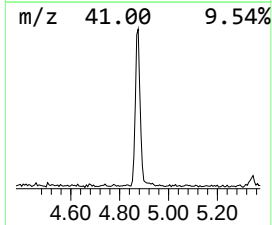
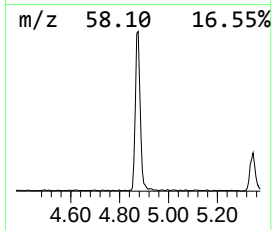
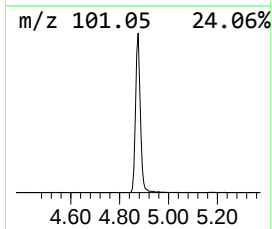
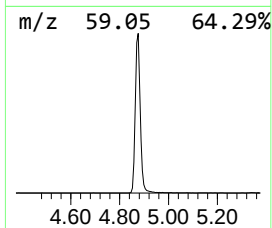
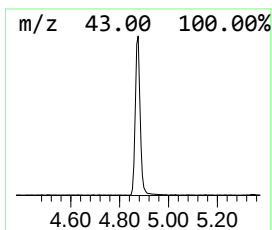
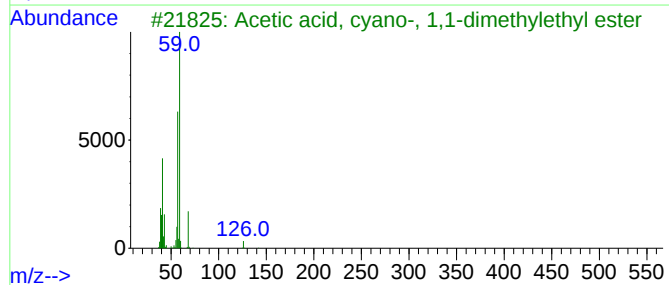
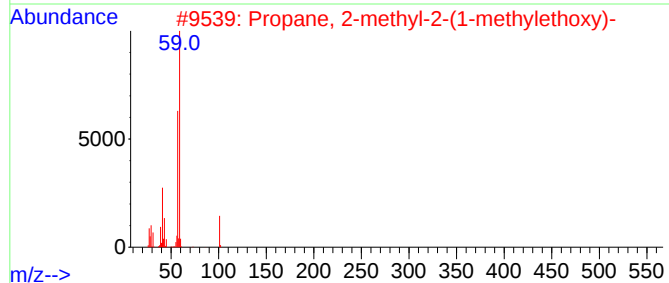
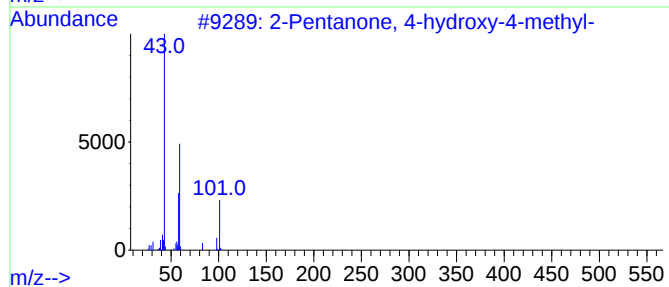
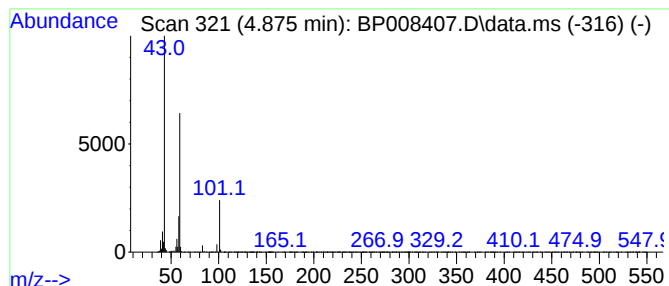
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.875	26.94 ng	442311	1,4-Dichlorobenzene-d4	7.746

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	50		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		



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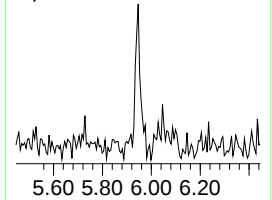
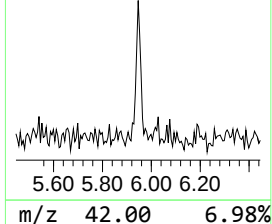
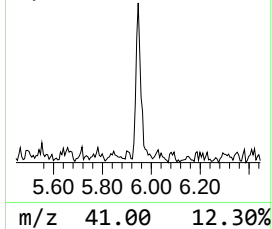
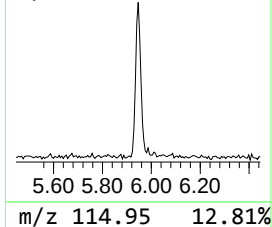
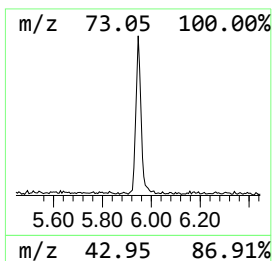
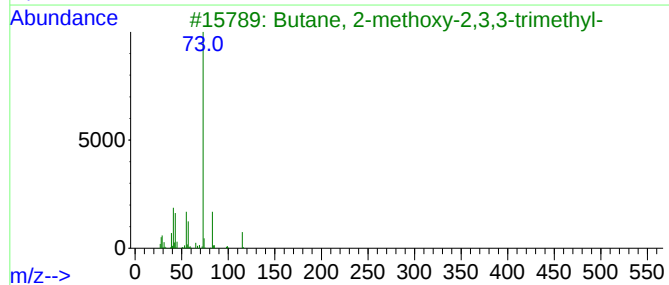
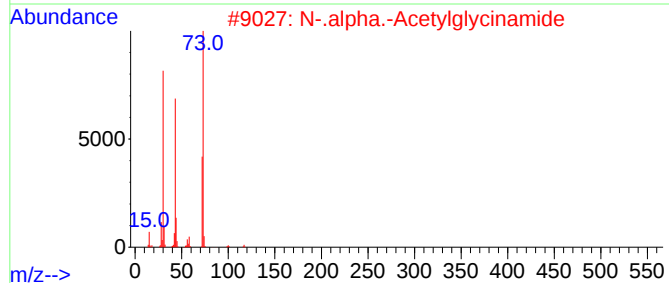
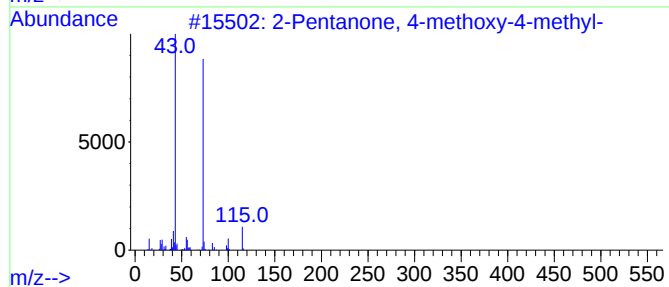
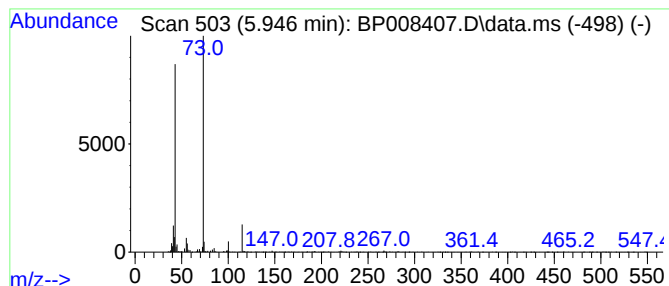
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.946	2.02 ng	33124	1,4-Dichlorobenzene-d4	7.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	59
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	27
3			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	12
4			1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	12
5			1,3-Dioxolane, 2-(6-heptynyl)-	168	C10H16O2	025595-82-8	10



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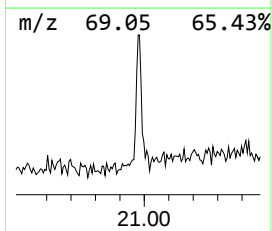
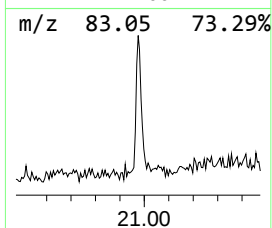
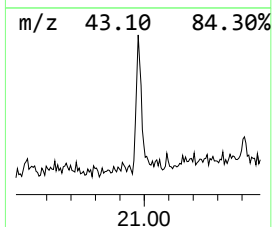
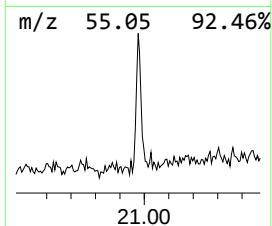
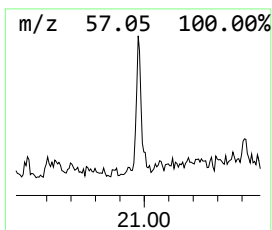
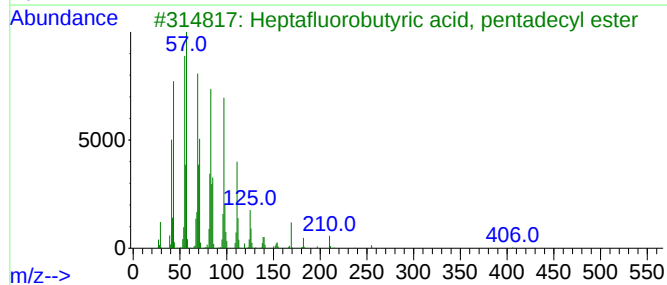
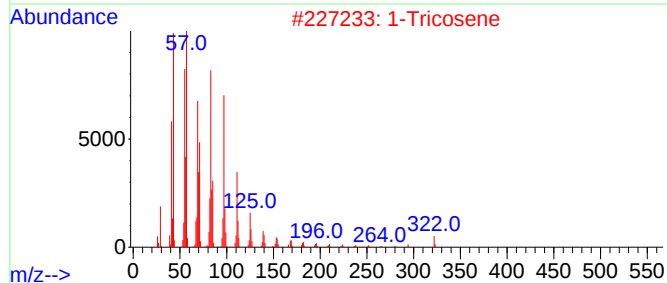
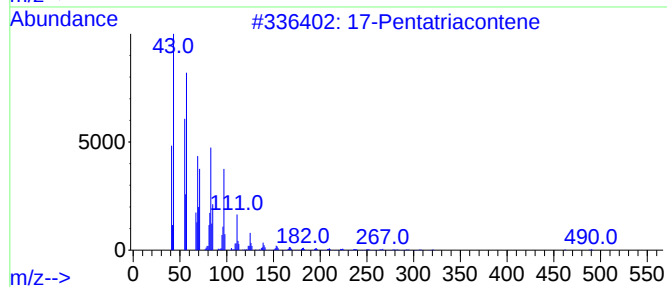
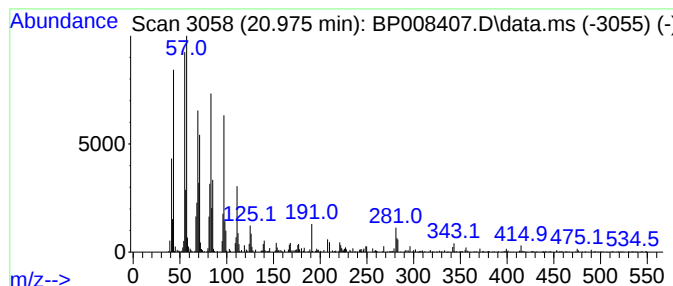
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Peak Number 3 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.975	2.45 ng	80043	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	95
2			1-Tricosene	322	C23H46	018835-32-0	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4			1-Triacontanol	438	C30H62O	000593-50-0	93
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90



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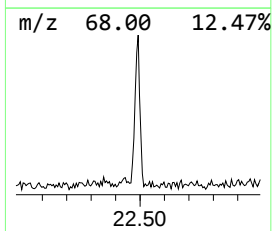
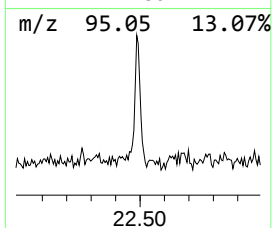
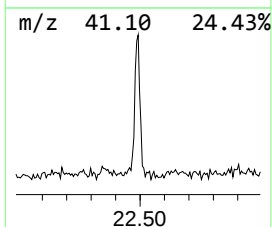
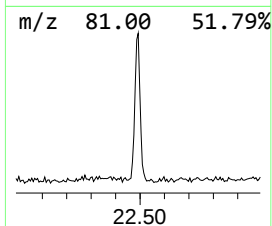
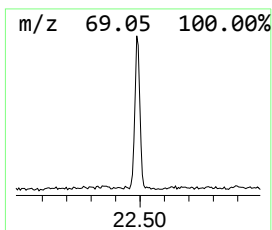
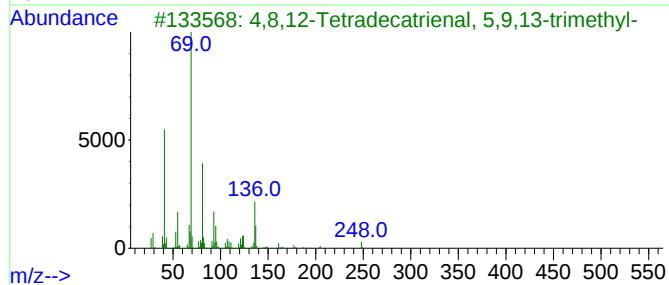
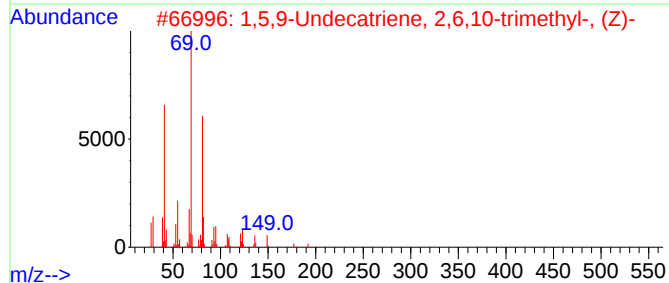
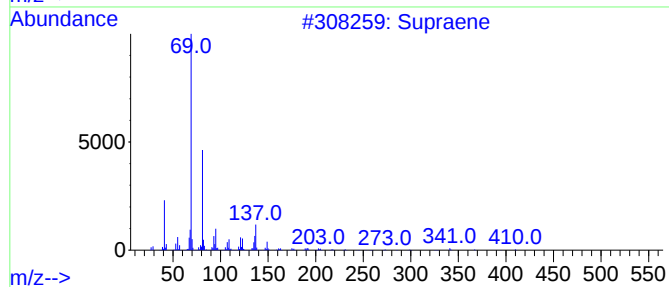
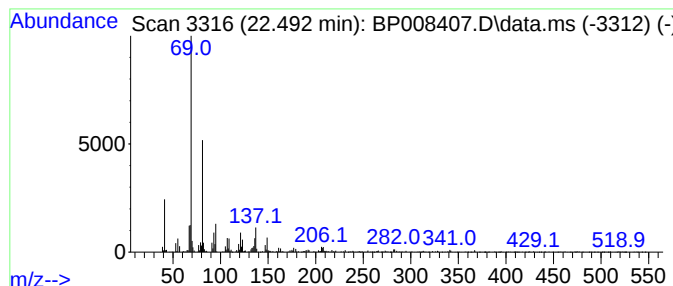
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Peak Number 4 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.492	4.72 ng	168910	Perylene-d12	23.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	96
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	90
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
4			Squalene	410	C30H50	000111-02-4	68
5			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.875	26.9	ng	442311	1	7.746	328333	20.0
2-Pentanone, 4-...	5.946	2.0	ng	33124	1	7.746	328333	20.0
17-Pentatriacon...	20.975	2.5	ng	80043	5	21.269	652109	20.0
Supraene	22.492	4.7	ng	168910	6	23.633	715724	20.0