

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
 Data File : BG060038.D
 Acq On : 15 Dec 2023 16:31
 Operator : MA/JU
 Sample : 05670-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-4

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060038.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.144	5	9	19	rVB	523101	816038	10.52%	3.345%
2	5.065	332	336	340	rVB	67525	98887	1.27%	0.405%
3	5.523	408	414	423	rVB	387935	612504	7.89%	2.510%
4	7.110	677	684	692	rBV2	226626	388811	5.01%	1.594%
5	7.956	821	828	834	rBV	218666	363523	4.68%	1.490%
6	9.119	1015	1026	1035	rBV	636543	1119645	14.43%	4.589%
7	10.764	1297	1306	1318	rBV	283338	520767	6.71%	2.134%
8	13.220	1715	1724	1733	rBV	2133221	3329651	42.91%	13.647%
9	14.595	1949	1958	1965	rBV	523131	822578	10.60%	3.371%
10	16.082	2203	2211	2219	rBV	2269365	3415705	44.02%	13.999%
11	17.345	2419	2426	2432	rBV	844400	1277130	16.46%	5.234%
12	18.232	2572	2577	2587	rBV2	187782	285385	3.68%	1.170%
13	19.965	2866	2872	2877	rBV	5850823	7759678	100.00%	31.803%
14	21.610	3147	3152	3160	rVB	1047634	1608964	20.73%	6.594%
15	23.303	3436	3440	3447	rVB3	176839	361124	4.65%	1.480%
16	24.807	3687	3696	3706	rVB2	591219	1618699	20.86%	6.634%

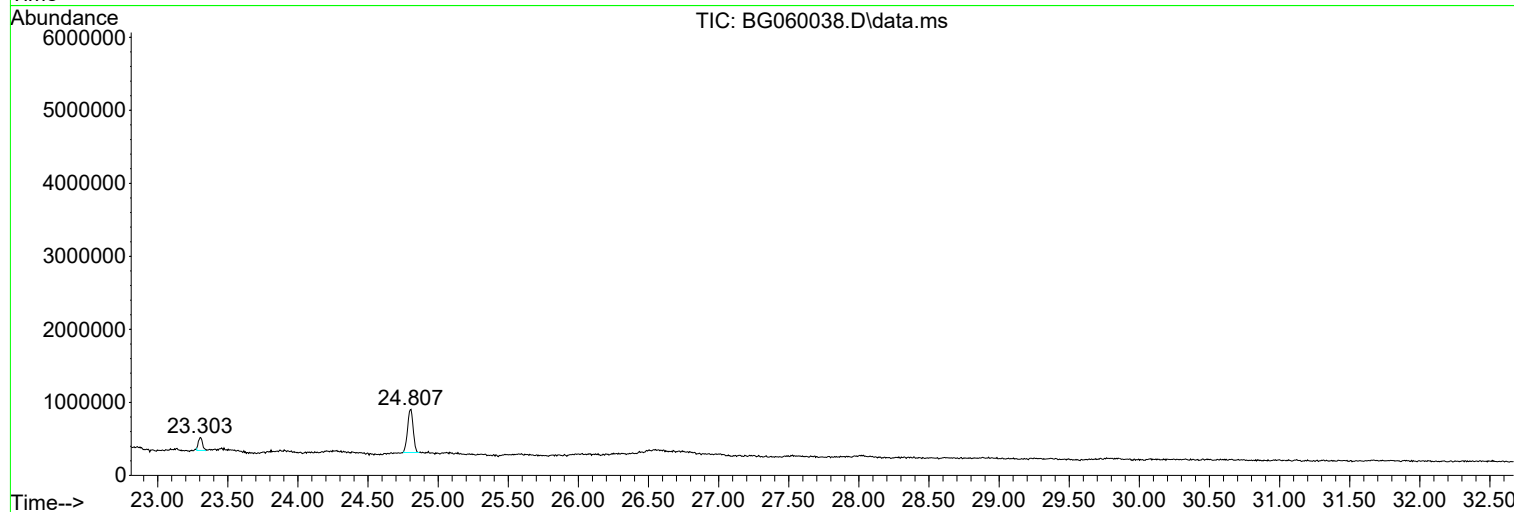
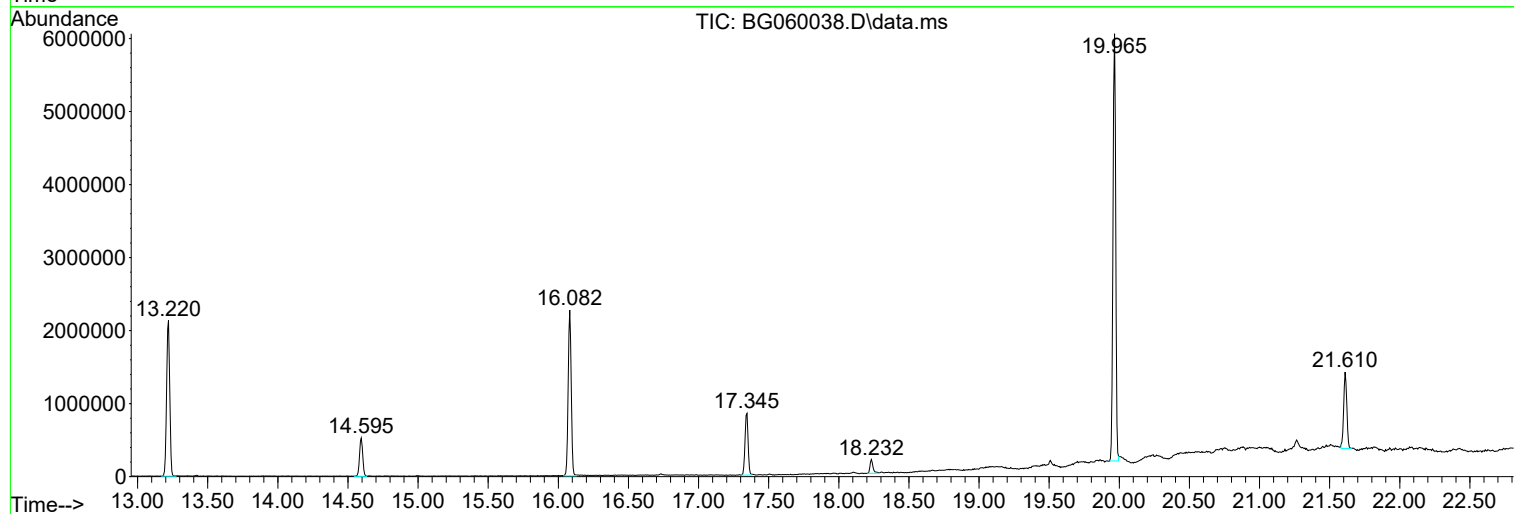
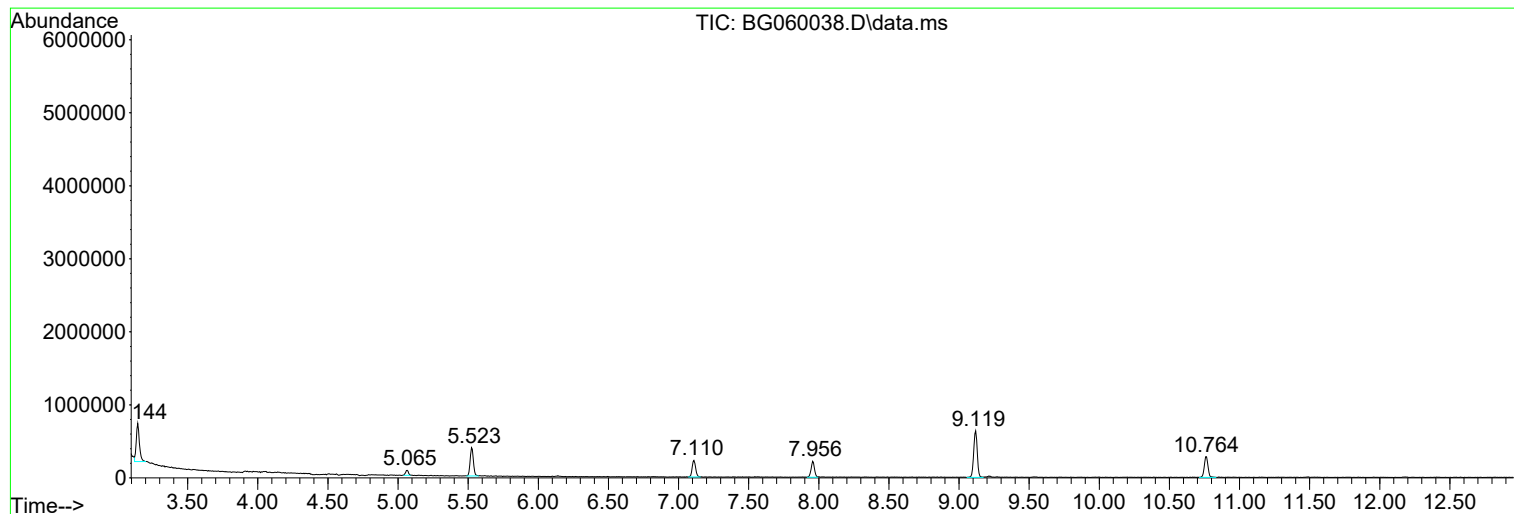
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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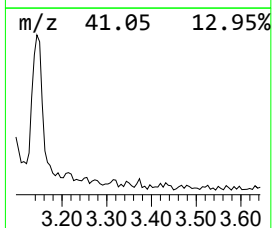
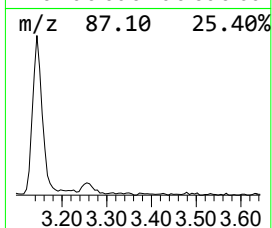
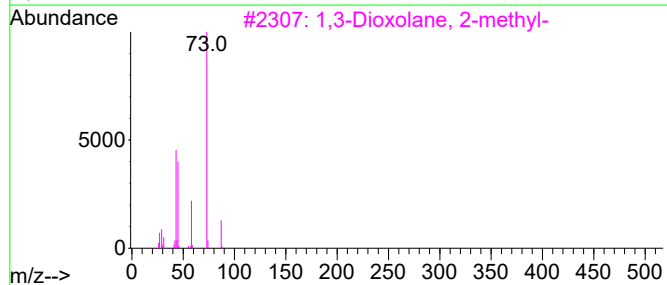
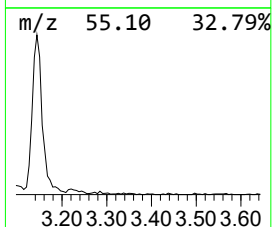
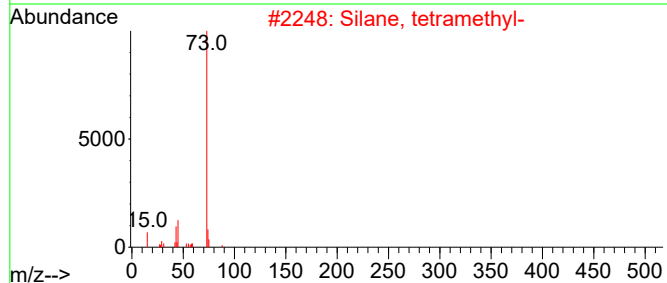
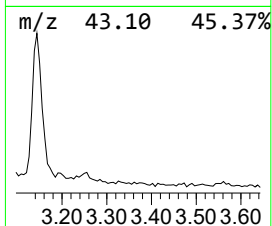
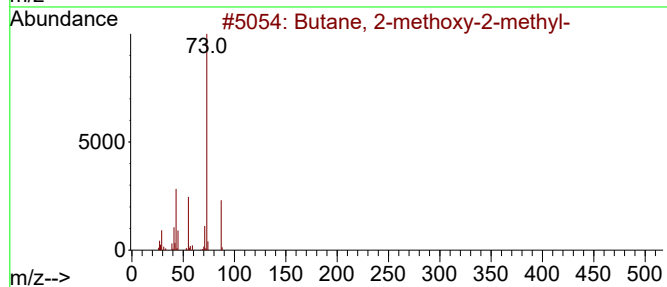
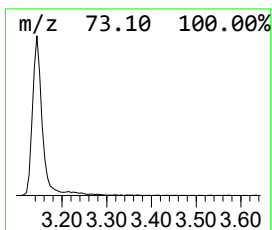
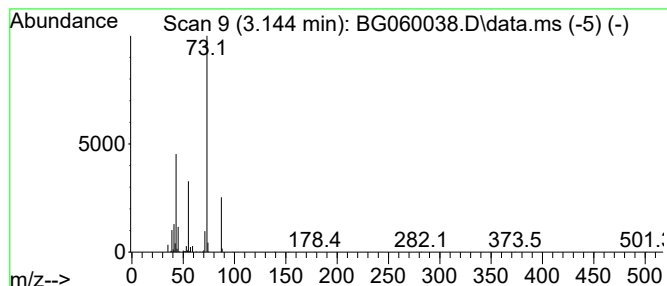
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.144	44.90 ng	816038	1,4-Dichlorobenzene-d4	7.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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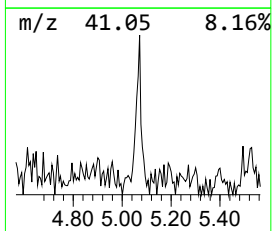
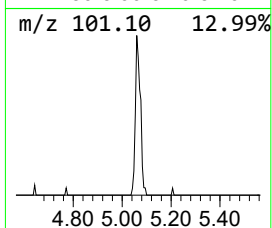
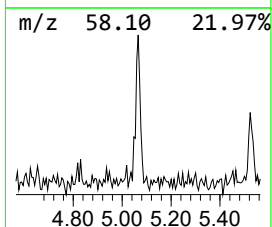
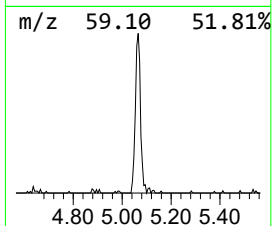
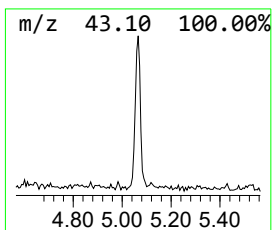
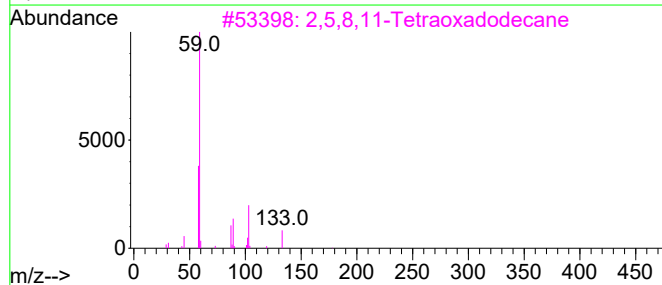
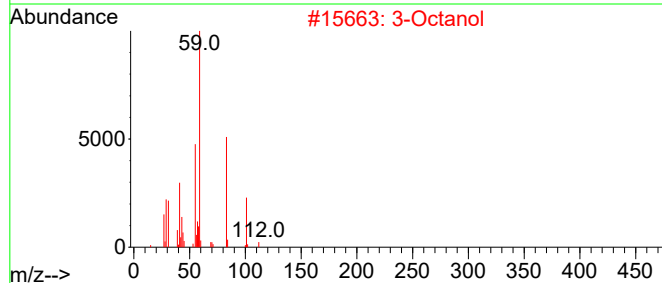
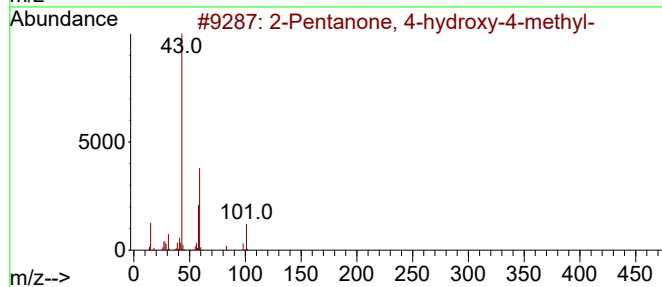
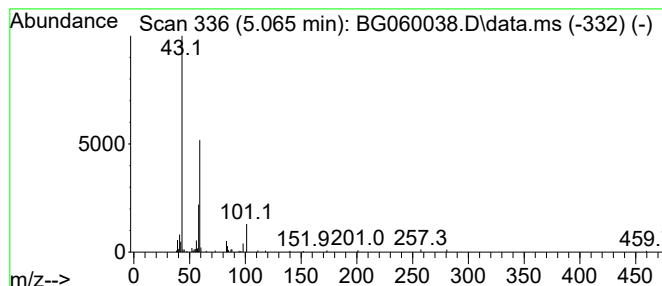
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
5.065	5.44 ng	98887	1,4-Dichlorobenzene-d4	7.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Octanol	130	C8H18O	000589-98-0	32
3			2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	25
4			4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	17
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12



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ClientSampleId :
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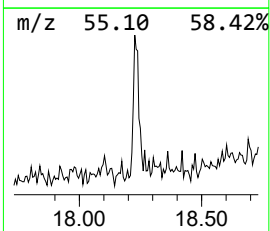
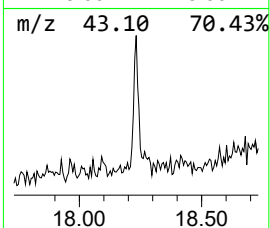
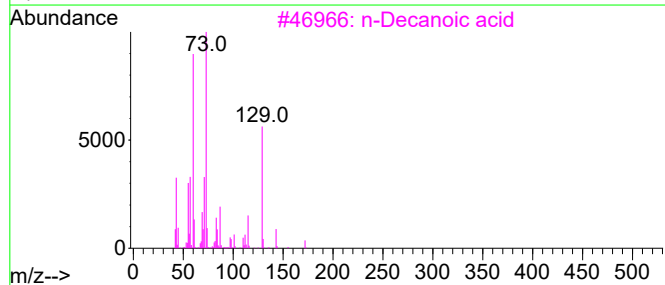
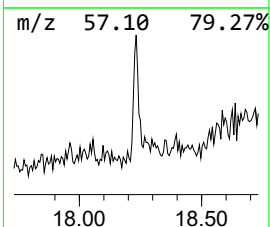
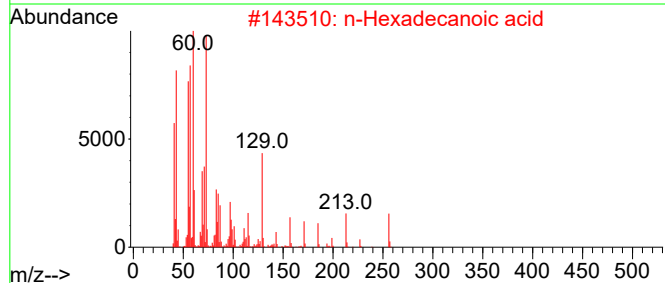
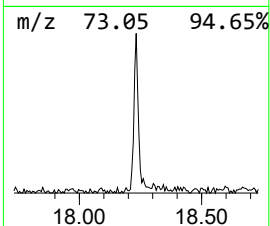
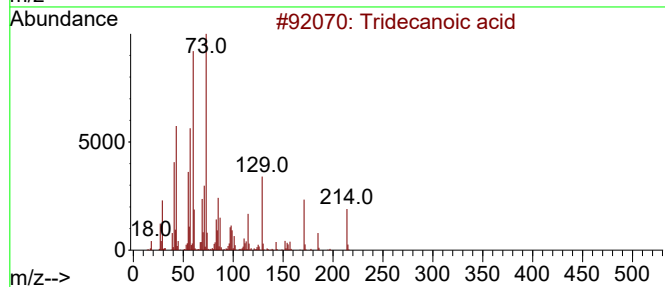
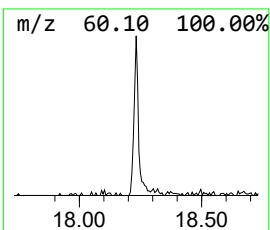
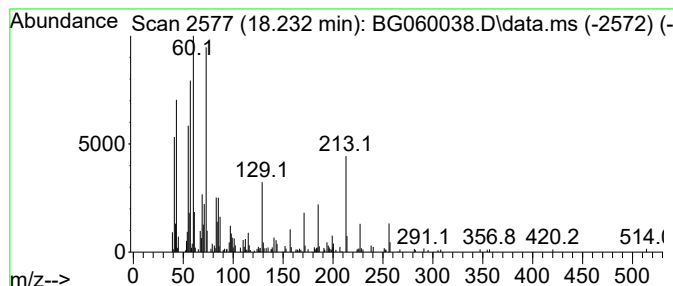
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Peak Number 3 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.232	4.47 ng	285385	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	92
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			n-Decanoic acid	172	C10H20O2	000334-48-5	64
4			Dodecanoic acid	200	C12H24O2	000143-07-7	55
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	53



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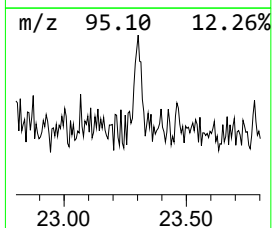
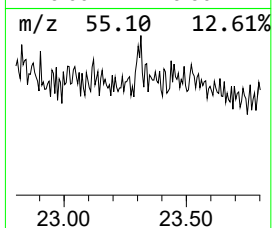
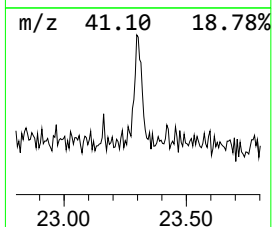
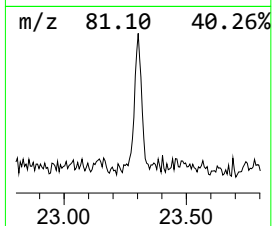
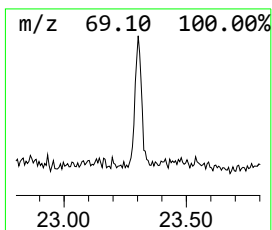
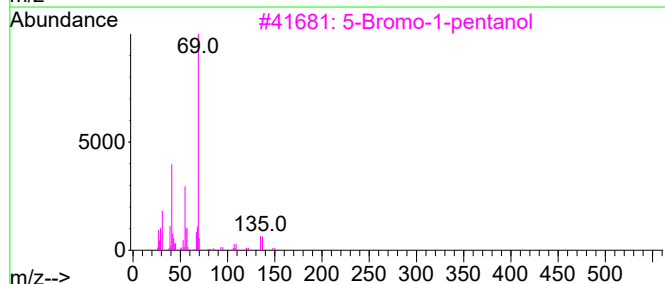
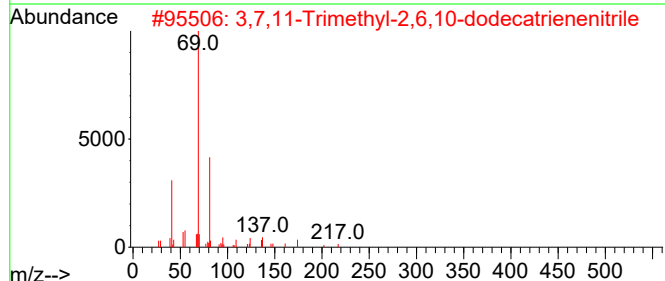
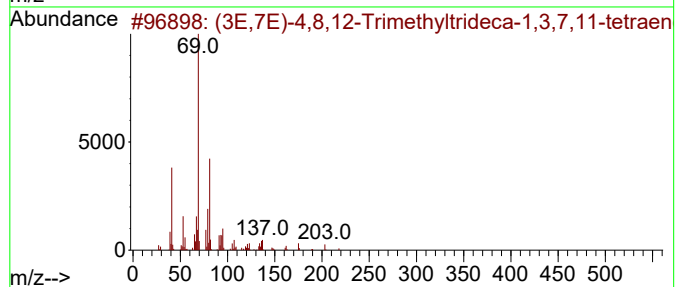
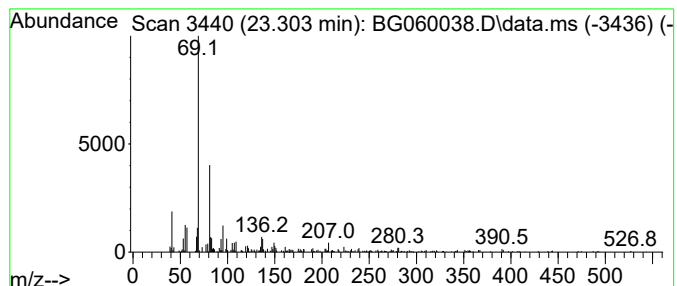
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Peak Number 4 (3E,7E)-4,8,12-Trimethyltri... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.303	4.46 ng	361124	Perylene-d12	24.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	72		
2	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59		
3	5-Bromo-1-pentanol	166	C5H11BrO	034626-51-2	59		
4	2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	003675-00-1	59		
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	50		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.144	44.9	ng	816038	1	7.956	363523	20.0
2-Pentanone, 4-...	5.065	5.4	ng	98887	1	7.956	363523	20.0
Tridecanoic acid	18.232	4.5	ng	285385	4	17.345	1277130	20.0
(3E,7E)-4,8,12-...	23.303	4.5	ng	361124	6	24.801	1618700	20.0