

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
 Data File : BG060135.D
 Acq On : 22 Dec 2023 12:49
 Operator : MA/JU
 Sample : 05898-07
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-71a

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-BG122123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.119	3	5	20	rVB	537473	809734	4.29%	0.986%
2	5.511	405	412	428	rBV	3744879	6439743	34.11%	7.844%
3	7.103	675	683	700	rBV	4373613	7785922	41.25%	9.484%
4	7.937	818	825	833	rBV	596538	1048426	5.55%	1.277%
5	9.101	1015	1023	1039	rBV	2563304	4606366	24.40%	5.611%
6	10.746	1296	1303	1315	rBV	921858	1700622	9.01%	2.071%
7	13.202	1713	1721	1734	rBV	7826773	12353822	65.44%	15.048%
8	14.577	1945	1955	1963	rBV	1911075	2965848	15.71%	3.613%
9	16.069	2200	2209	2221	rBV	6443128	10240239	54.25%	12.473%
10	17.326	2416	2423	2434	rBV	2558104	3969944	21.03%	4.836%
11	18.214	2569	2574	2584	rBV2	548343	833129	4.41%	1.015%
12	19.947	2862	2869	2880	rBV	13571044	18876775	100.00%	22.993%
13	21.239	3083	3089	3097	rBV	838144	1355610	7.18%	1.651%
14	21.586	3142	3148	3161	rVB2	2007310	3399794	18.01%	4.141%
15	22.397	3279	3286	3296	rBV4	339982	893216	4.73%	1.088%
16	23.919	3540	3545	3555	rVB2	328818	758888	4.02%	0.924%
17	24.765	3678	3689	3701	rBV2	1136652	3225131	17.09%	3.928%
18	25.916	3879	3885	3894	rVB4	110830	284271	1.51%	0.346%
19	26.046	3898	3907	3919	rVV4	166419	550365	2.92%	0.670%

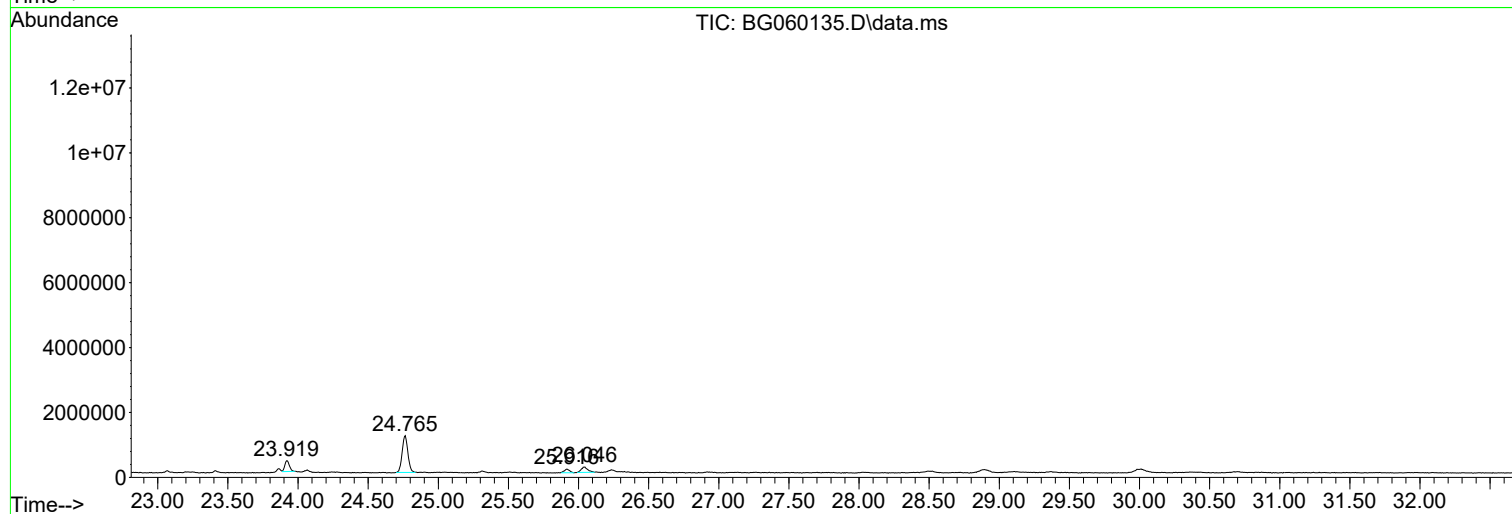
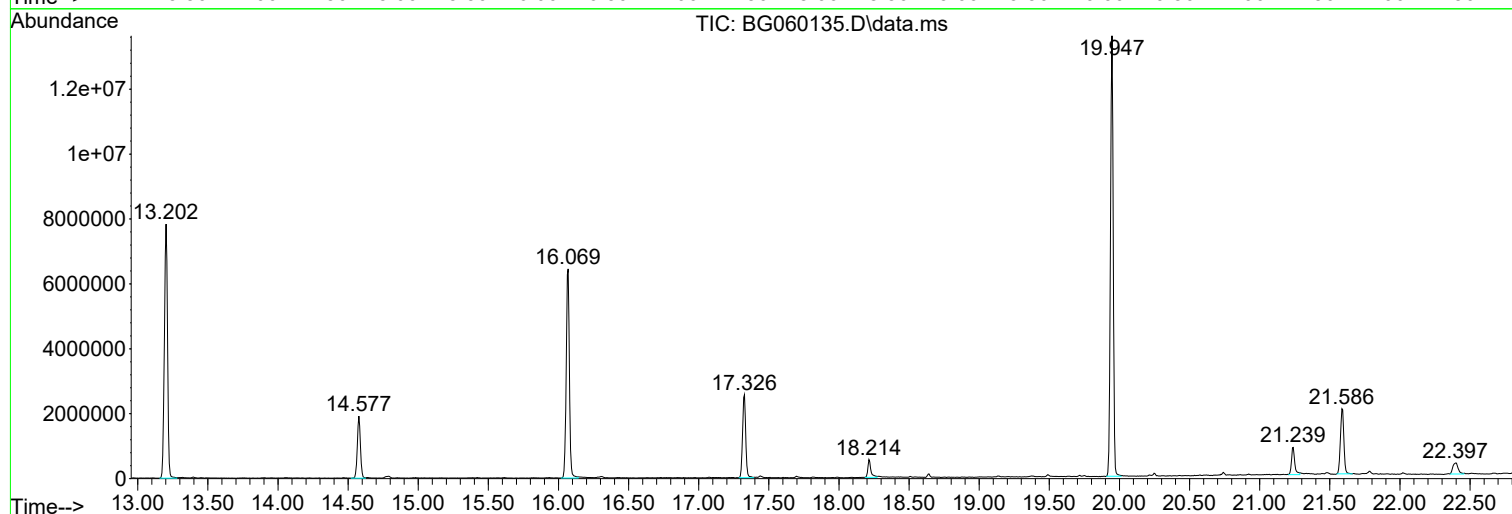
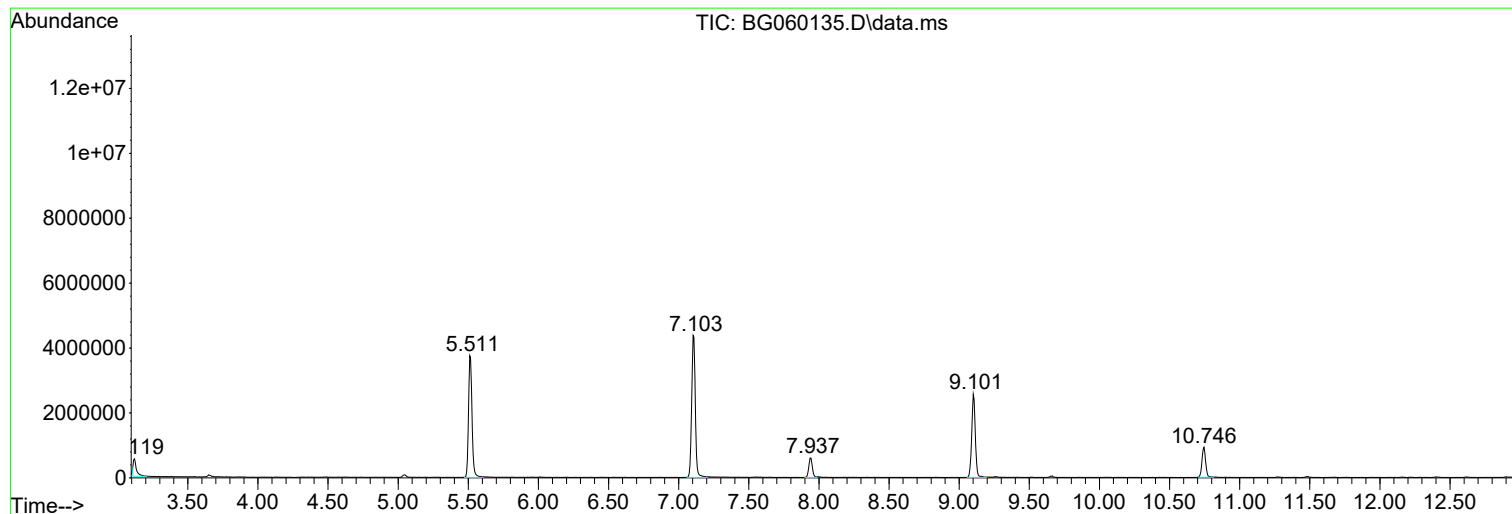
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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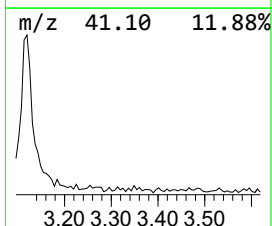
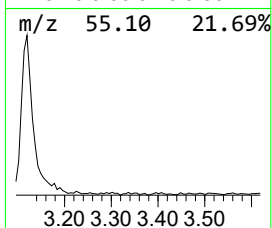
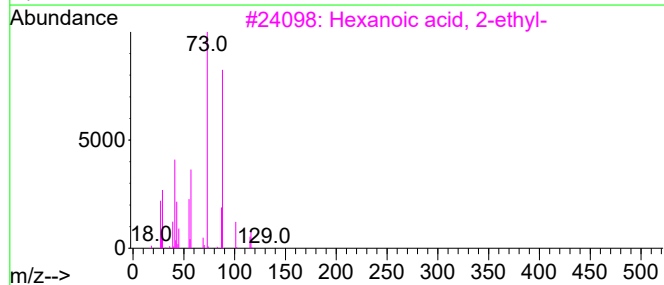
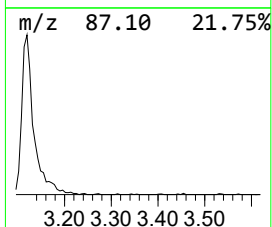
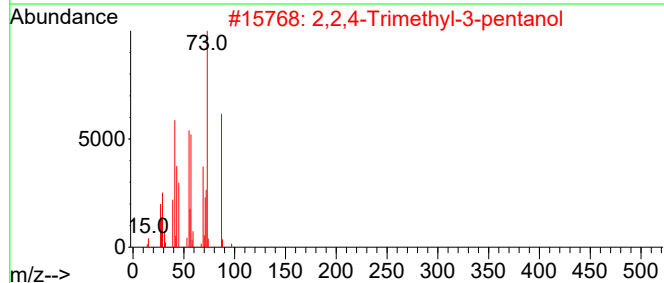
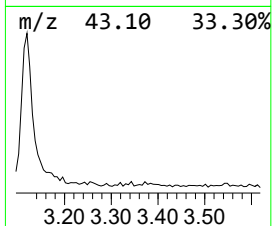
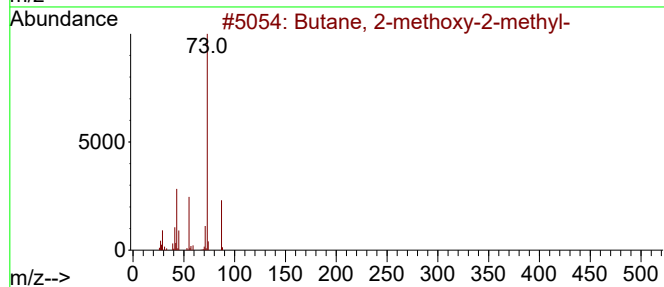
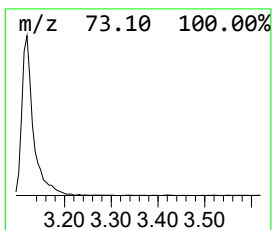
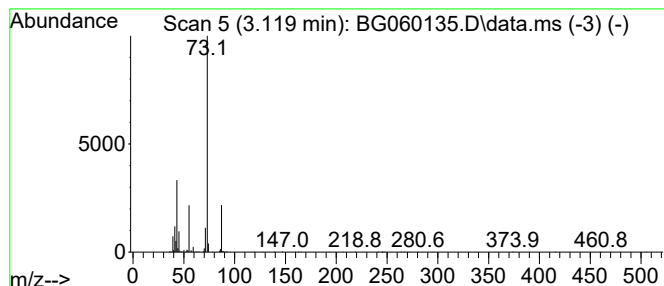
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.119	15.45 ng	809734	1,4-Dichlorobenzene-d4	7.943

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	33
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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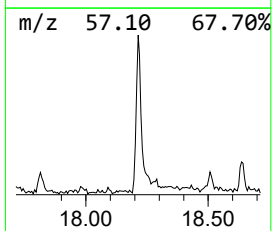
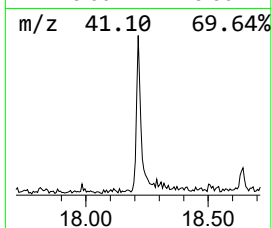
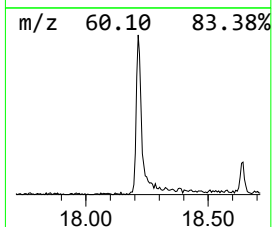
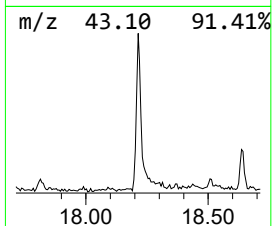
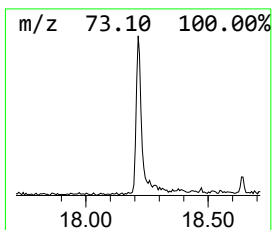
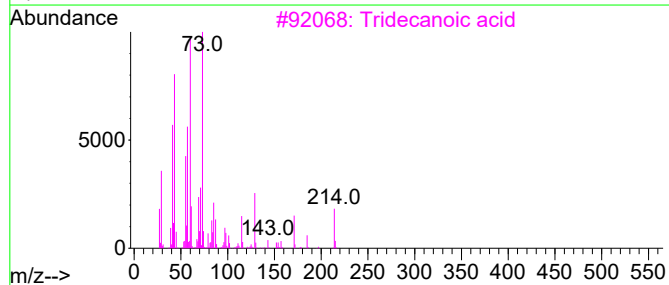
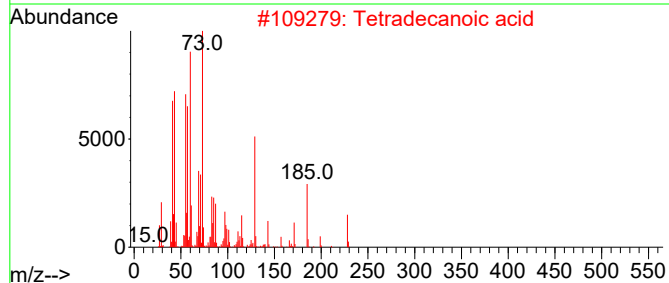
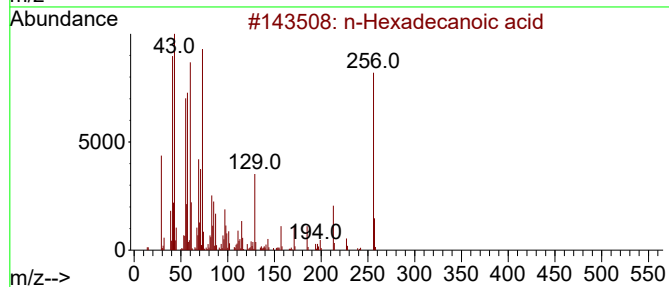
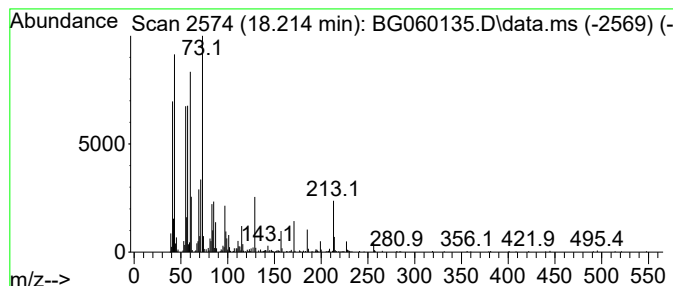
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.214	4.20 ng	833129	Phenanthrene-d10	17.326

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Isopropyl palmitate	298	C19H38O2	000142-91-6	72
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	72



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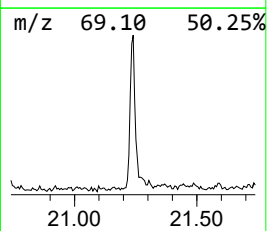
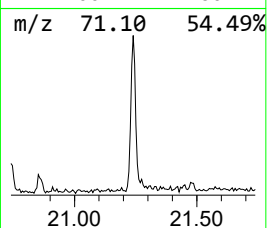
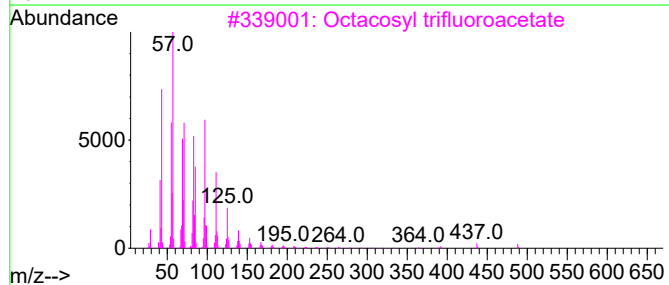
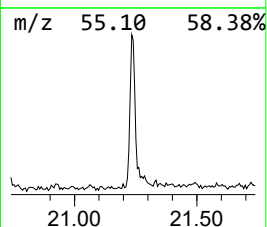
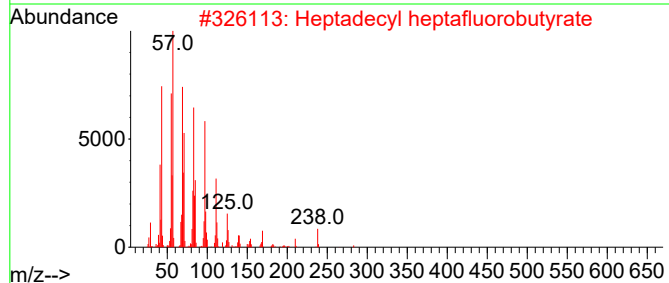
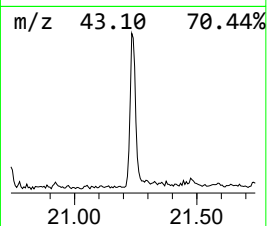
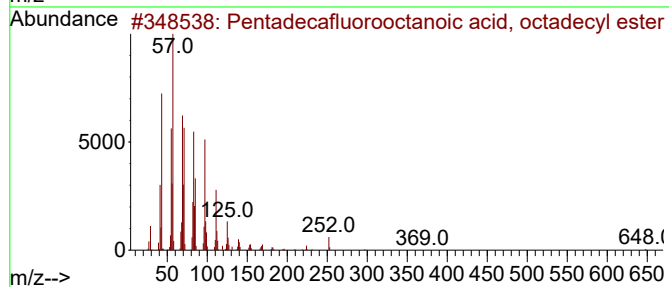
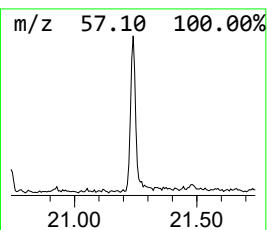
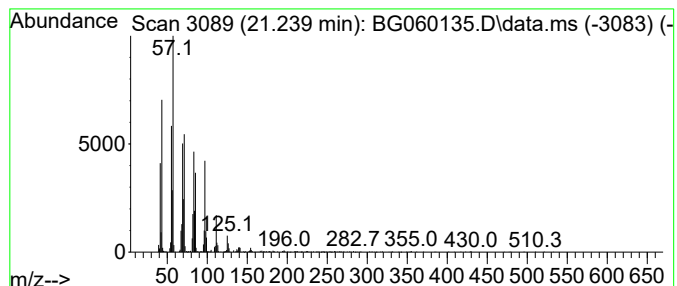
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Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.239	7.97 ng	1355610	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90



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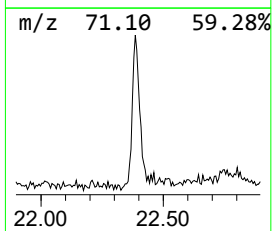
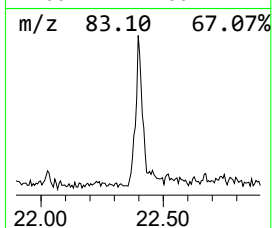
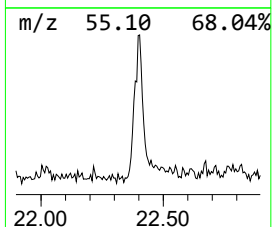
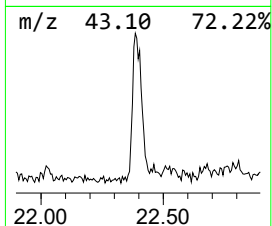
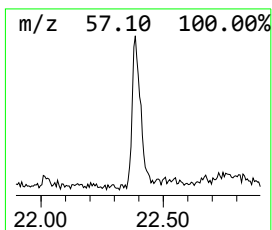
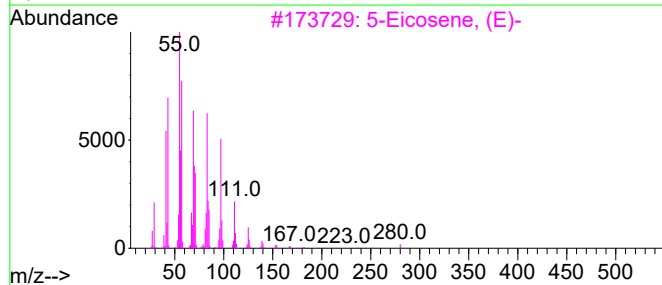
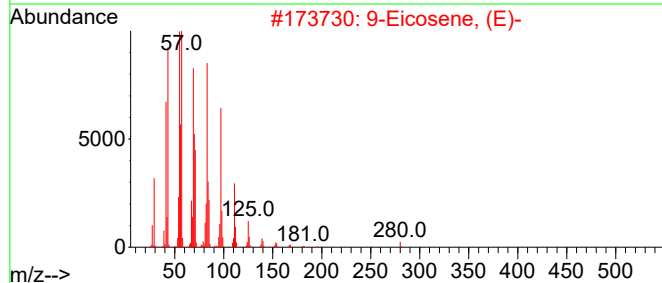
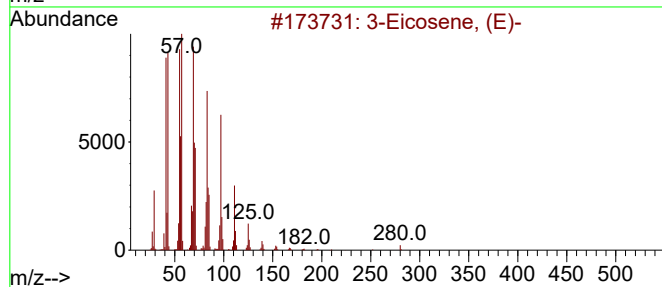
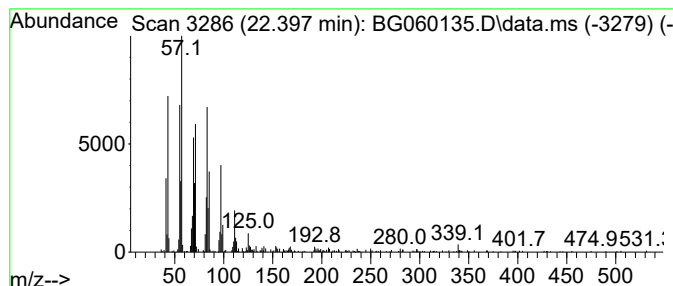
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.397	5.25 ng	893216	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	93
2			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	87
4			Trihexadecyl borate	735	C48H99B03	002665-11-4	87
5			Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	83



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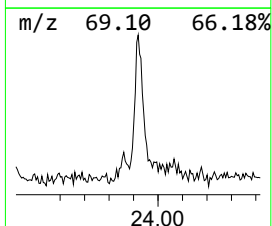
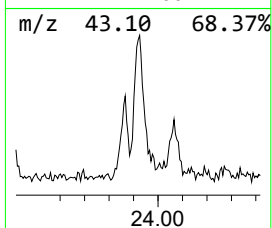
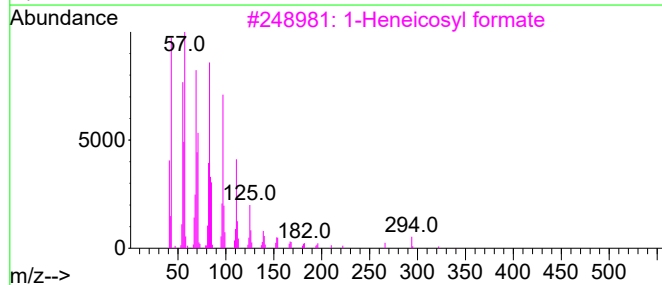
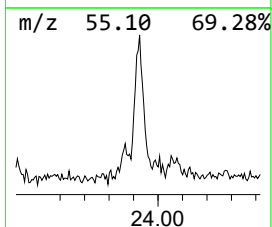
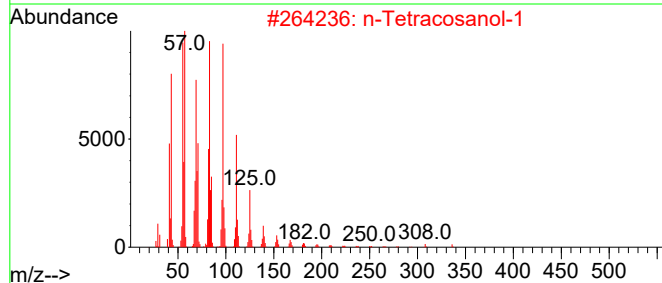
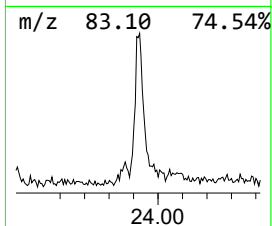
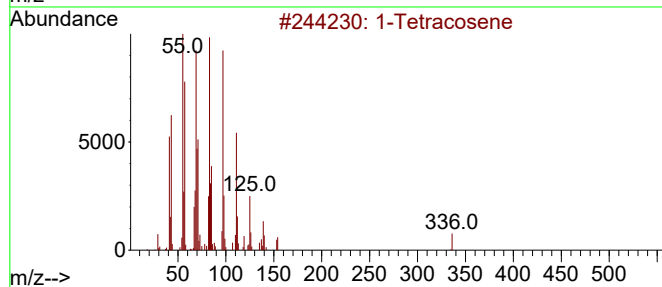
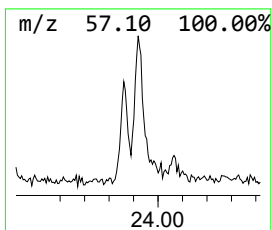
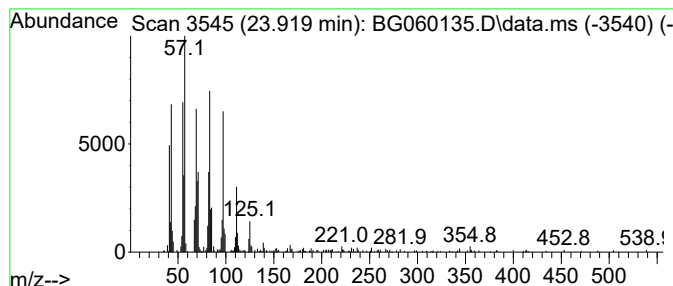
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Peak Number 5 1-Tetracosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.919	4.71 ng	758888	Perylene-d12	24.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	97
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4			Octacosanol	410	C28H58O	000557-61-9	91
5			1-Nonadecene	266	C19H38	018435-45-5	91



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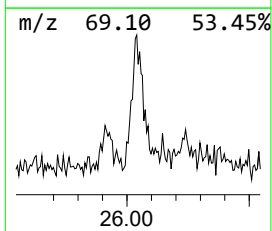
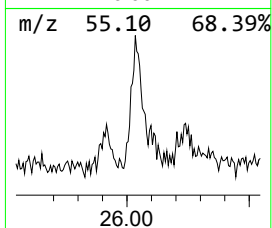
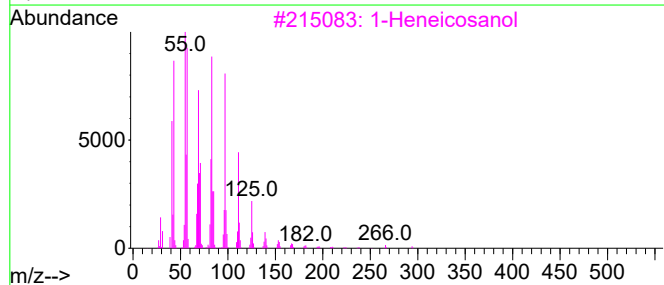
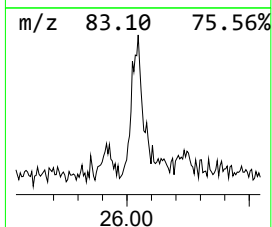
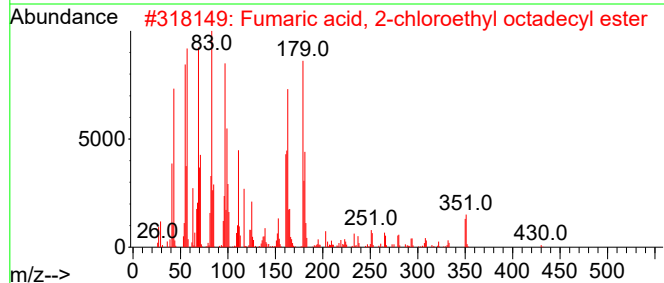
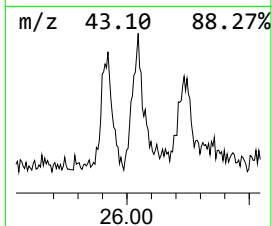
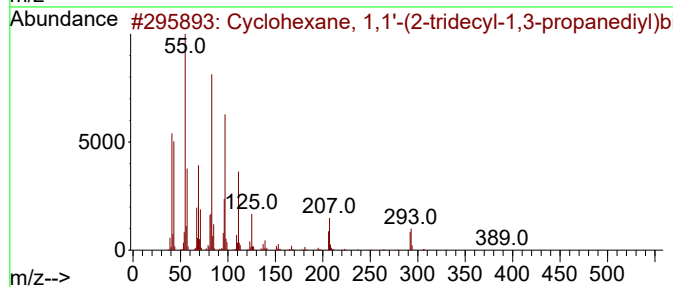
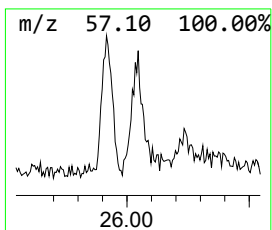
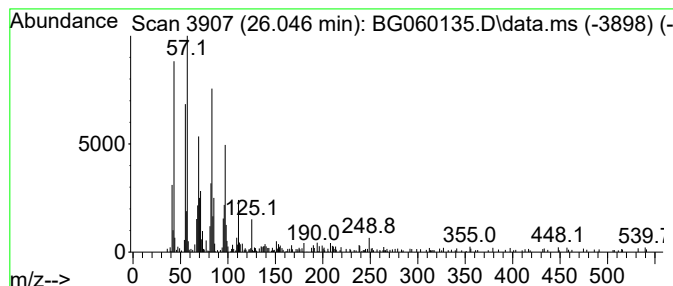
Instrument :
BNA_G
ClientSampleId :
GHL-SS-71a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexane, 1,1'-(2-tridec... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.046	3.41 ng	550365	Perylene-d12	24.765	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1'-(2-tridecyl-1,...	390	C28H54	055255-74-8	80
2	Fumaric acid, 2-chloroethyl octa...	430	C24H43ClO4	1000330-62-4	72
3	1-Heneicosanol	312	C21H44O	015594-90-8	72
4	Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	68
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060135.D
Acq On : 22 Dec 2023 12:49
Operator : MA/JU
Sample : 05898-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-71a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.119	15.4	ng	809734	1	7.943	1048430	20.0
n-Hexadecanoic ...	18.214	4.2	ng	833129	4	17.326	3969940	20.0
Pentadecafluoro...	21.239	8.0	ng	1355610	5	21.586	3399790	20.0
3-Eicosene, (E)-	22.397	5.3	ng	893216	5	21.586	3399790	20.0
1-Tetracosene	23.919	4.7	ng	758888	6	24.765	3225130	20.0
Cyclohexane, 1,...	26.046	3.4	ng	550365	6	24.765	3225130	20.0