

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
 Data File : BG048031.D
 Acq On : 27 Jan 2021 15:55
 Operator : CG/JU
 Sample : M1244-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FB-BP24

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-BG012521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048031.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.679	391	398	407	rVB	489036	776238	17.79%	3.908%
2	7.271	661	669	681	rBV	303960	575505	13.19%	2.897%
3	8.123	808	814	821	rBV	177350	301347	6.91%	1.517%
4	9.286	1004	1012	1022	rBV	665219	1177697	27.00%	5.929%
5	10.937	1284	1293	1300	rVB	247515	440371	10.09%	2.217%
6	13.376	1701	1708	1717	rVB	1923952	2923676	67.02%	14.720%
7	14.192	1840	1847	1851	rBV	99237	145673	3.34%	0.733%
8	14.745	1935	1941	1951	rVB2	454635	716256	16.42%	3.606%
9	15.138	2004	2008	2014	rBV3	31840	46403	1.06%	0.234%
10	16.231	2185	2194	2205	rBV	1825467	2754033	63.13%	13.866%
11	17.489	2401	2408	2415	rBV	619022	918776	21.06%	4.626%
12	18.370	2548	2558	2568	rBV	556741	847223	19.42%	4.266%
13	19.140	2685	2689	2694	rBV	82100	95612	2.19%	0.481%
14	19.492	2746	2749	2751	rBV2	41543	53450	1.23%	0.269%
15	19.633	2769	2773	2783	rBV	386317	567567	13.01%	2.858%
16	19.768	2793	2796	2803	rVB3	26982	44165	1.01%	0.222%
17	20.091	2845	2851	2857	rVB	3393701	4362553	100.00%	21.964%
18	20.773	2964	2967	2972	rVB2	51239	68995	1.58%	0.347%
19	20.996	3000	3005	3009	rBV	197753	261376	5.99%	1.316%
20	21.037	3009	3012	3017	rVB2	47136	59355	1.36%	0.299%
21	21.402	3069	3074	3083	rVB5	164428	295822	6.78%	1.489%
22	21.478	3083	3087	3093	rVB	85707	124317	2.85%	0.626%
23	21.554	3098	3100	3107	rVB4	35432	48279	1.11%	0.243%
24	21.766	3130	3136	3145	rVB2	566621	957533	21.95%	4.821%
25	21.966	3167	3170	3177	rVB3	45871	69897	1.60%	0.352%
26	22.583	3272	3275	3286	rVB5	45595	104856	2.40%	0.528%
27	23.299	3393	3397	3405	rVB3	52240	93472	2.14%	0.471%
28	24.128	3534	3538	3545	rVB2	58739	111234	2.55%	0.560%
29	25.044	3685	3694	3703	rBV2	326279	920522	21.10%	4.635%

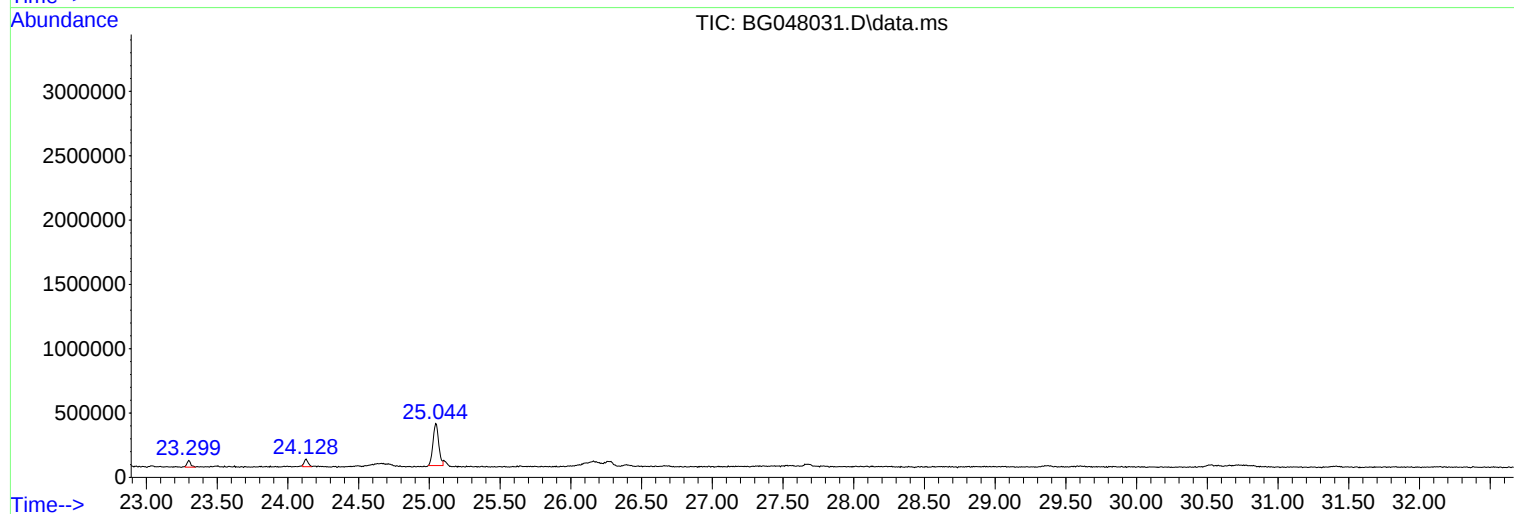
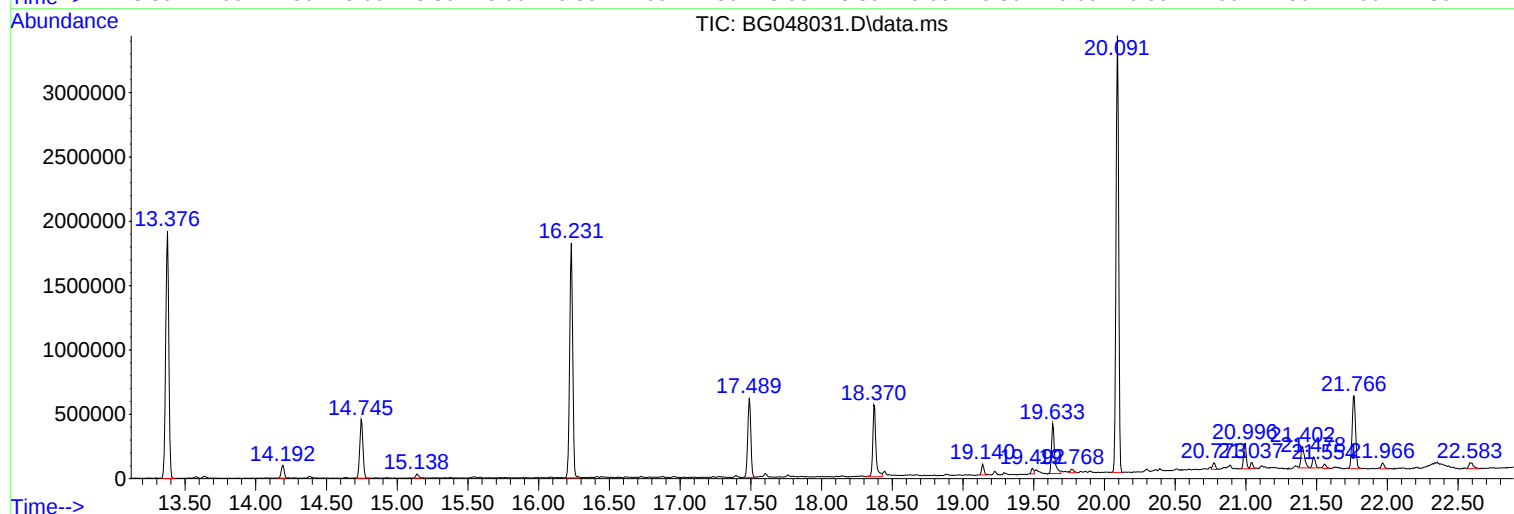
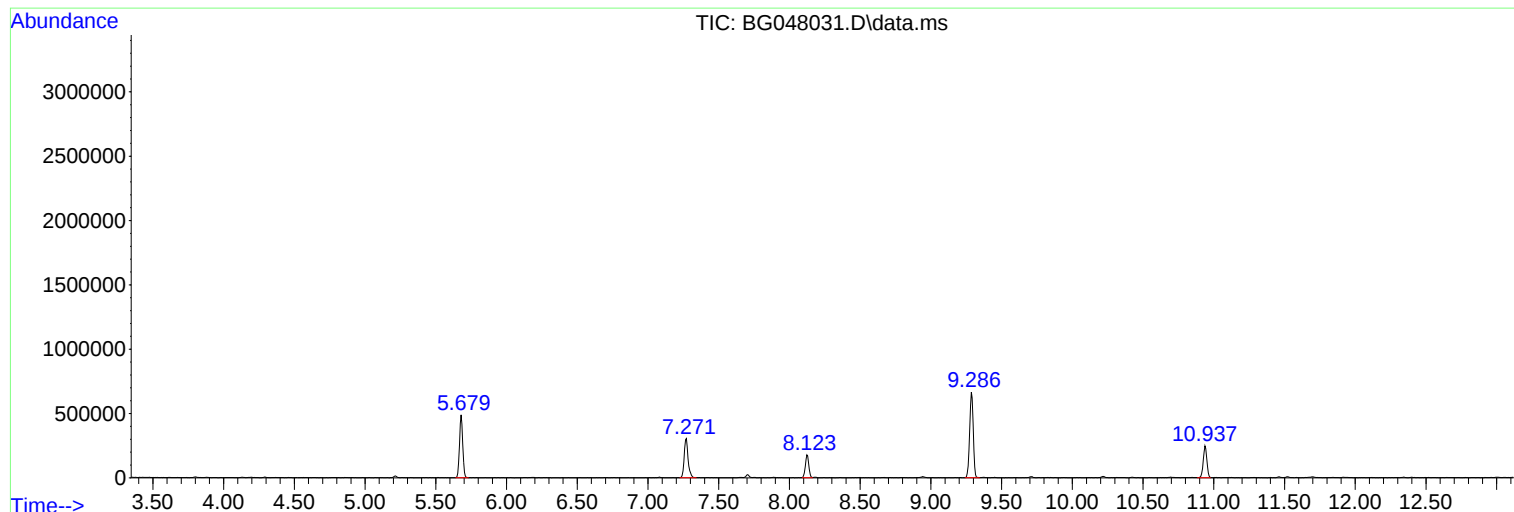
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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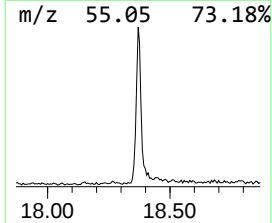
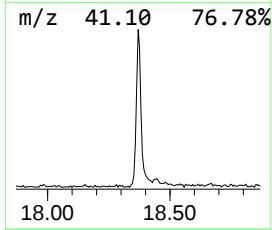
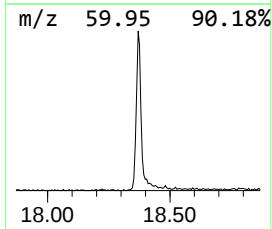
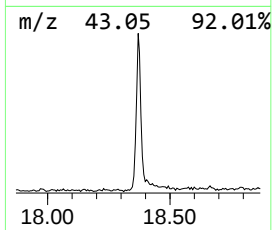
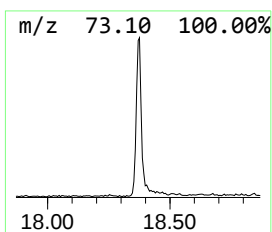
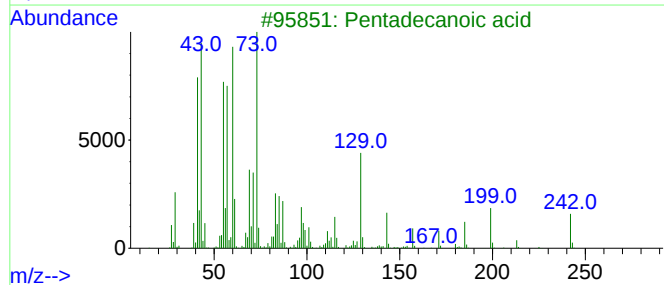
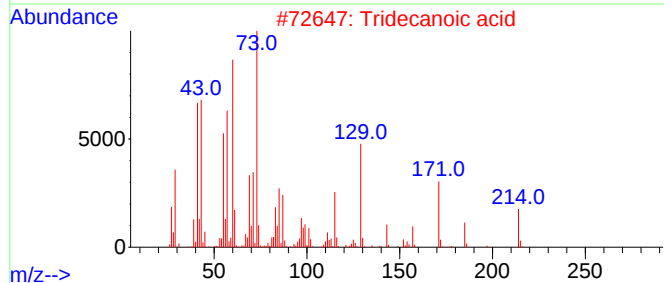
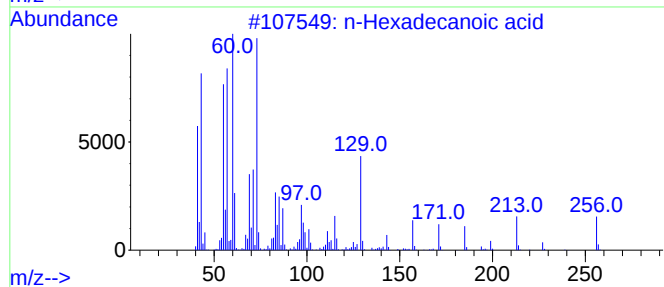
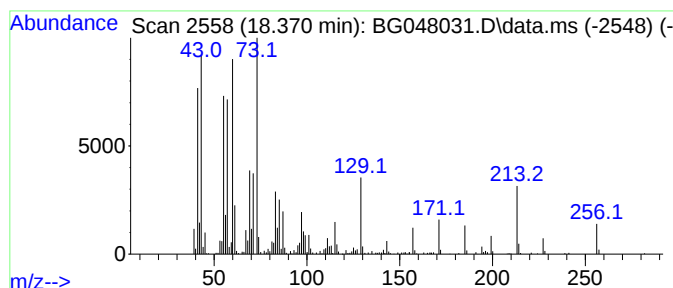
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.370	18.44 ng	847223	Phenanthrene-d10	17.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Octanoic acid	144	C8H16O2	000124-07-2	47



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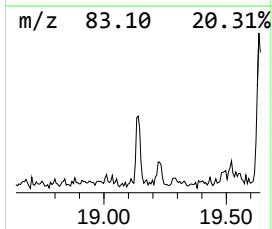
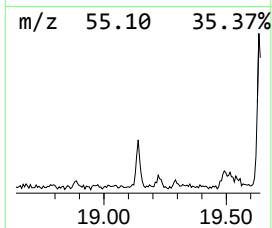
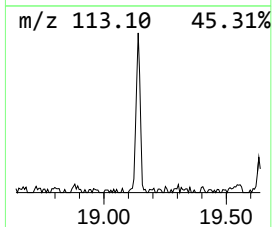
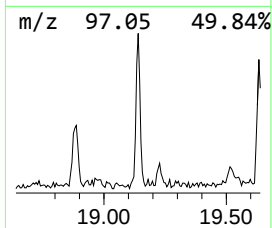
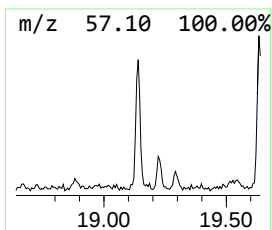
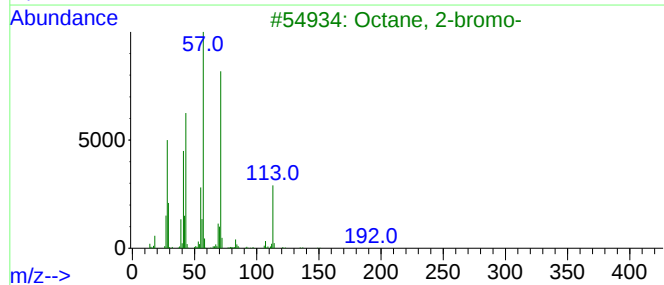
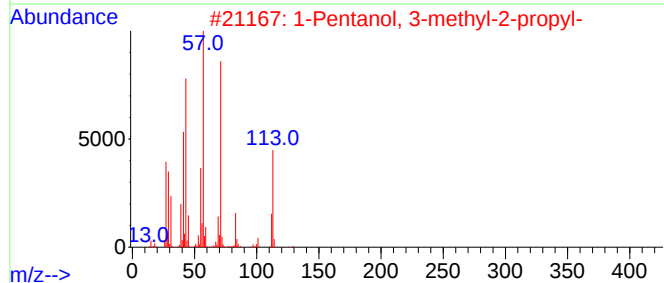
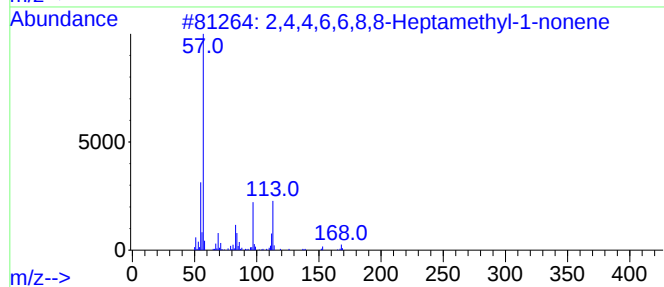
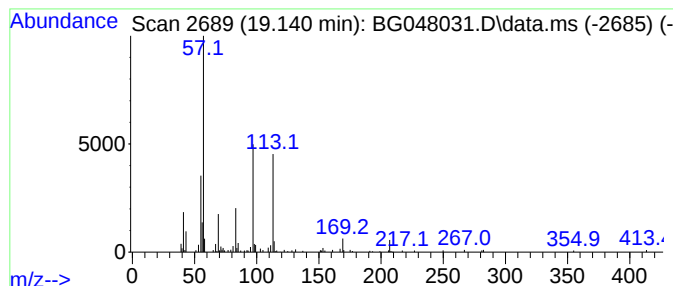
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Peak Number 2 unknown19.14 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.140	2.08 ng	95612	Phenanthrene-d10	17.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	53		
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	37		
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35		
4	4-Methylnonanoic acid	172	C10H20O2	045019-28-1	28		
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25		



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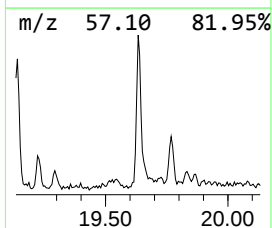
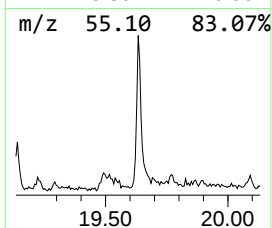
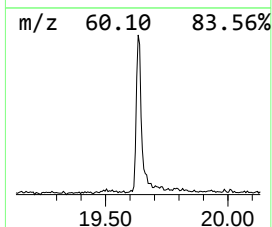
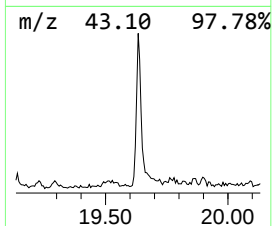
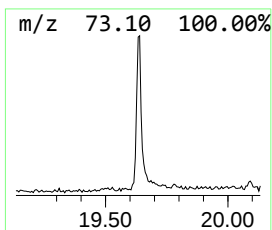
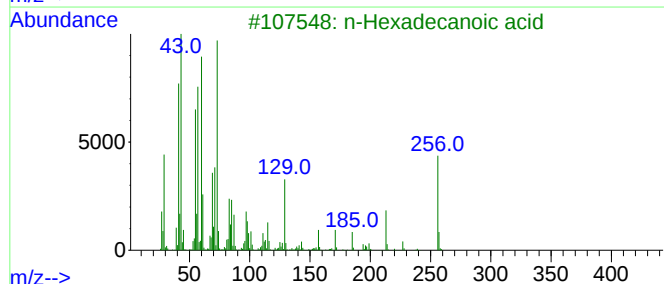
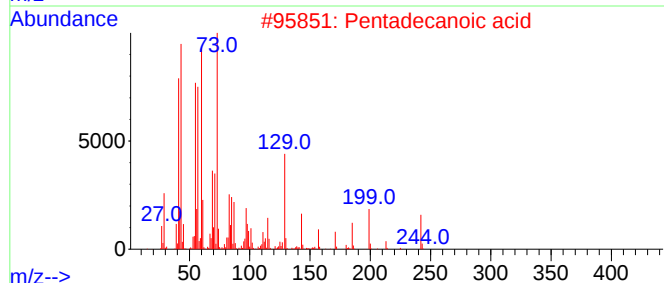
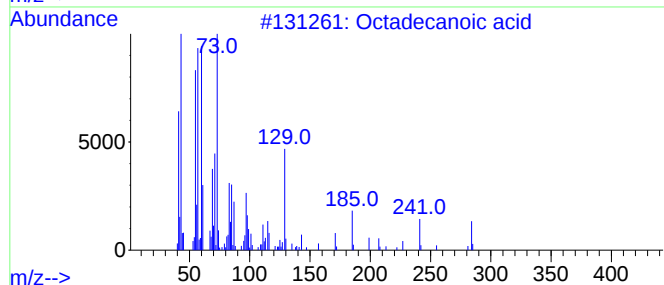
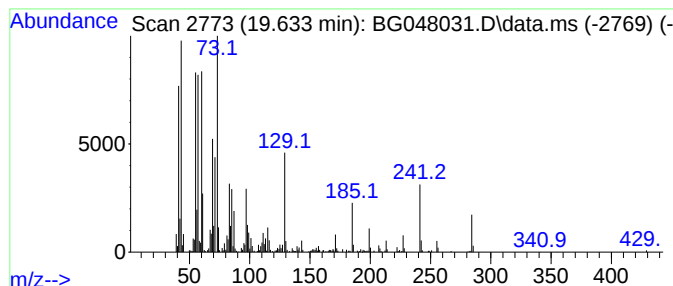
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ClientSampleId :
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.633	11.85 ng	567567	Chrysene-d12		21.766	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	86
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	83
5	Tridecanoic acid		214	C13H26O2	000638-53-9	68



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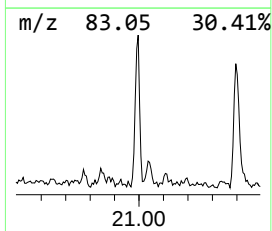
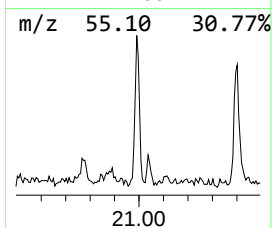
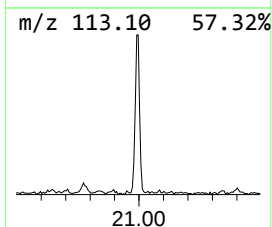
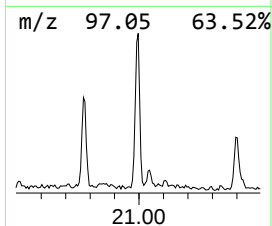
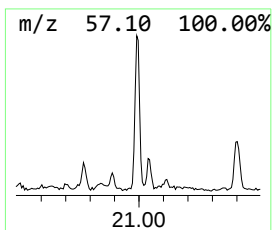
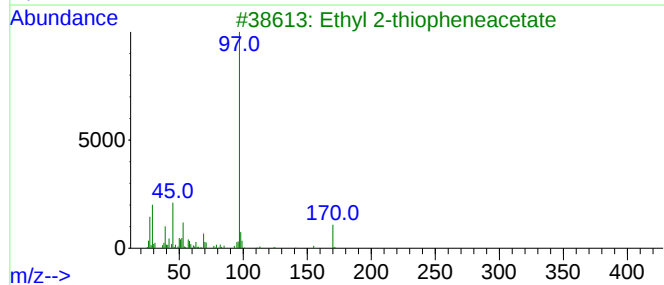
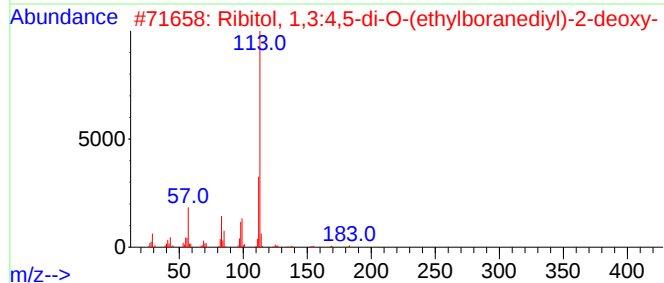
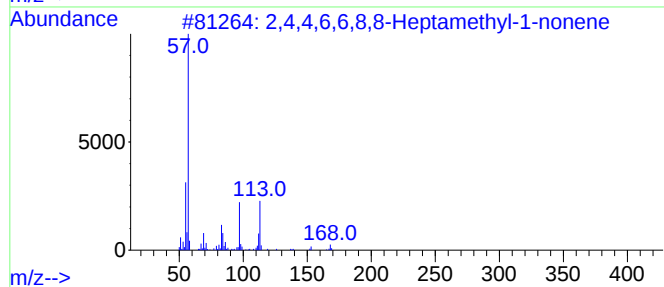
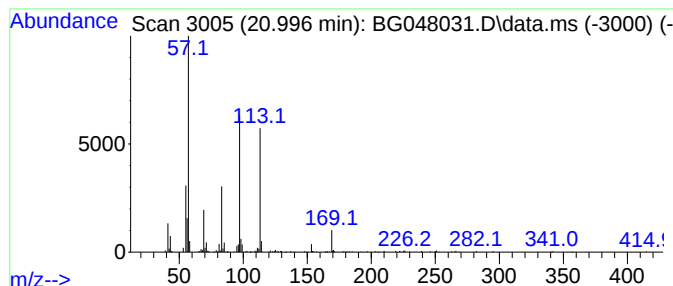
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Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.996	5.46 ng	261376	Chrysene-d12	21.766

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32		015796-04-0	56
2	Ribitol, 1,3:4,5-di-O-(ethylbora...	212	C9H18B2O4		1000149-52-8	16
3	Ethyl 2-thiopheneacetate	170	C8H10O2S		057382-97-5	14
4	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2		1000365-19-5	14
5	Thiophene, 2-pentyl-	154	C9H14S		004861-58-9	14



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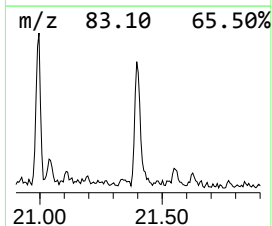
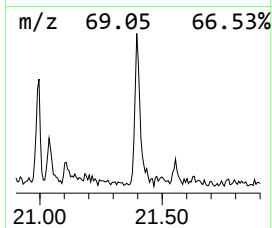
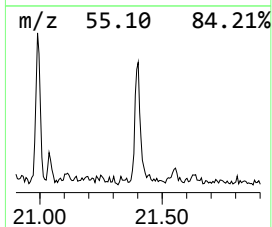
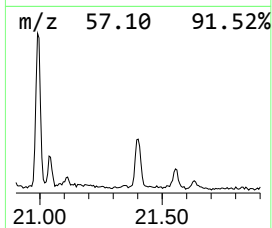
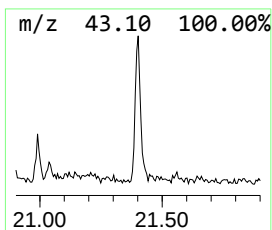
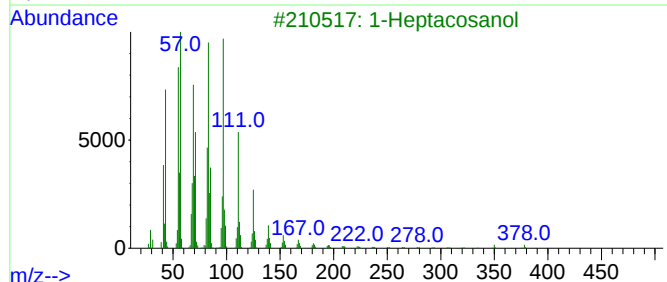
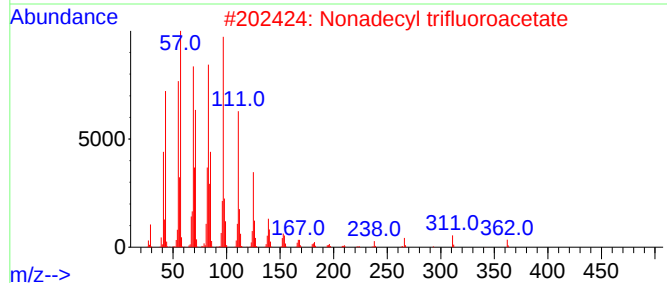
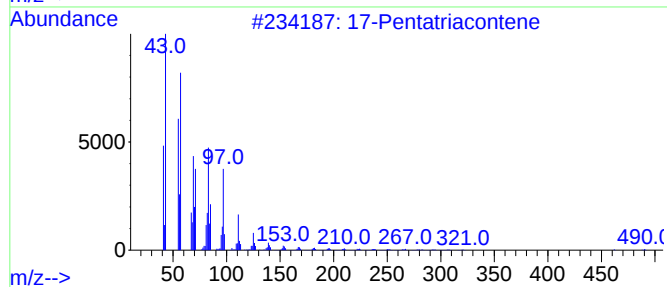
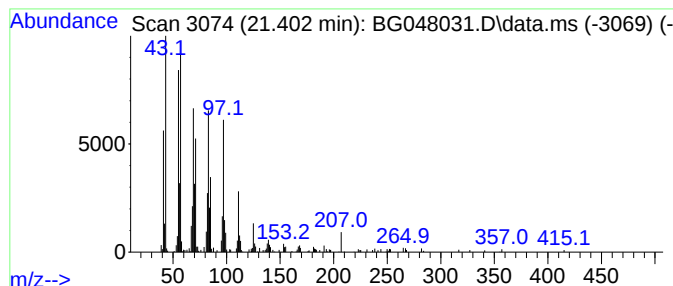
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Peak Number 5 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.402	6.18 ng	295822	Chrysene-d12	21.766

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5			Heptadecafluorononanoic acid, he...	702	C26H35F17O2	1000356-03-3	91



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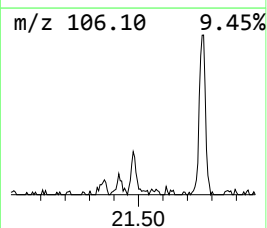
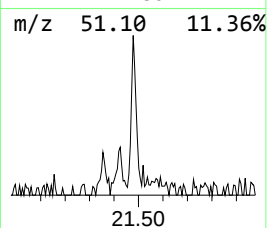
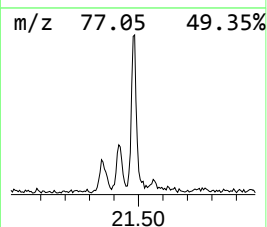
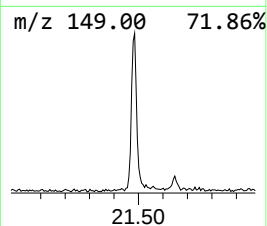
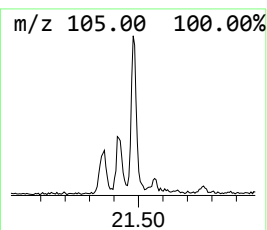
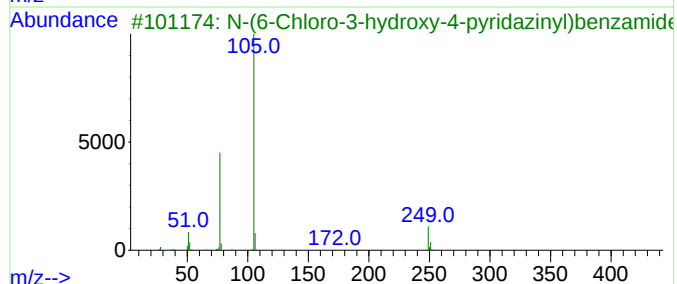
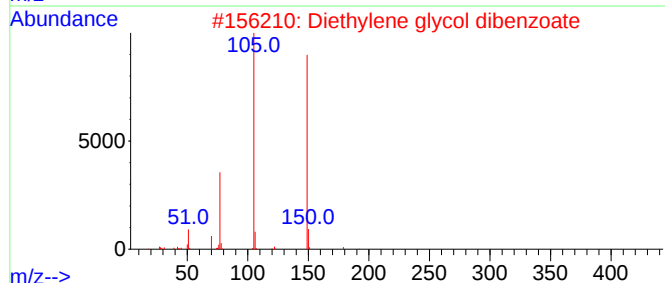
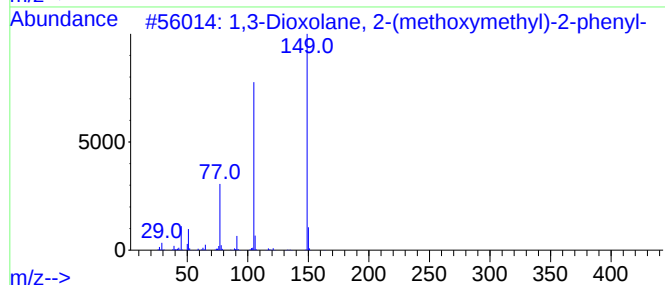
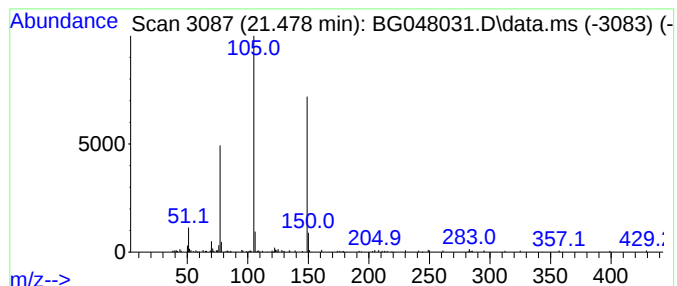
Instrument :
BNA_G
ClientSampleId :
FB-BP24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.478	2.60 ng	124317	Chrysene-d12	21.766	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59
3	N-(6-Chloro-3-hydroxy-4-pyridazi...	249	C11H8ClN3O2	117892-39-4	49
4	1,3-Phenylenedibenzoate	318	C20H14O4	000094-01-9	47
5	Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048031.D
Acq On : 27 Jan 2021 15:55
Operator : CG/JU
Sample : M1244-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

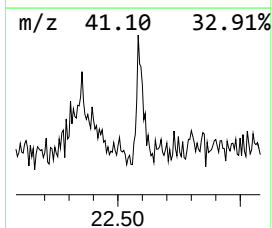
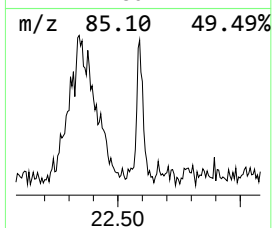
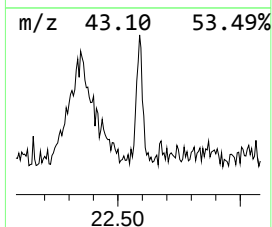
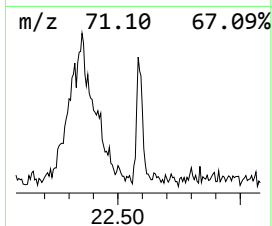
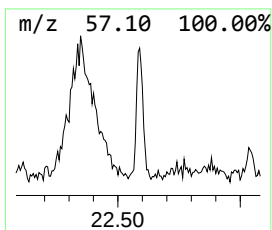
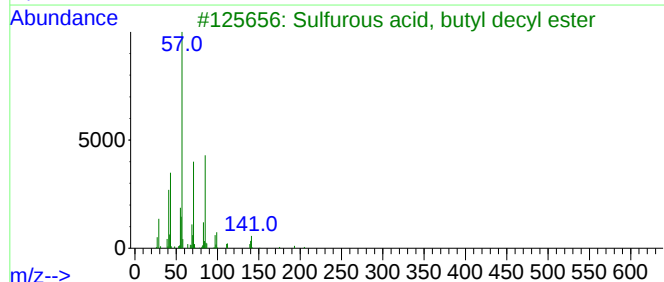
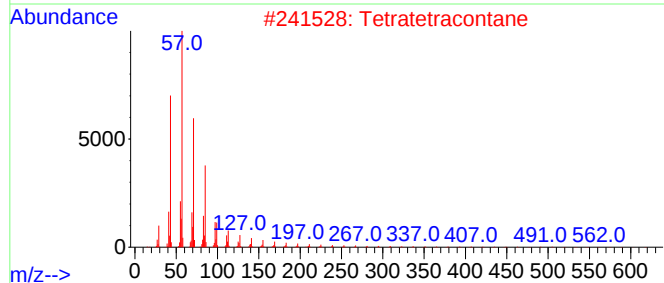
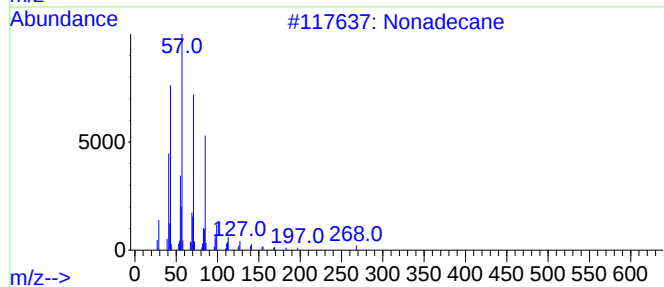
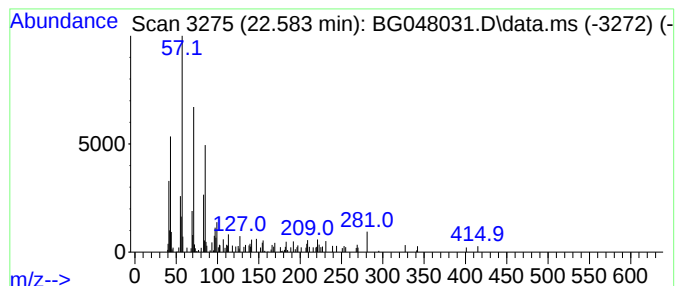
Instrument :
BNA_G
ClientSampleId :
FB-BP24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.583	2.19 ng	104856	Chrysene-d12		21.766	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	86
2	Tetratetracontane		619	C44H90	007098-22-8	68
3	Sulfurous acid, butyl decyl ester		278	C14H30O3S	1000309-17-7	64
4	Tetracosane		338	C24H50	000646-31-1	64
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048031.D
Acq On : 27 Jan 2021 15:55
Operator : CG/JU
Sample : M1244-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB-BP24

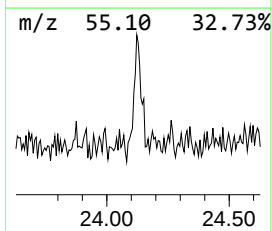
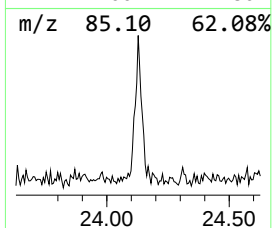
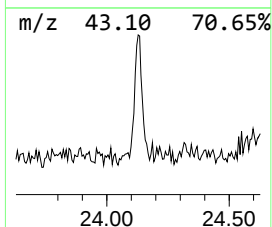
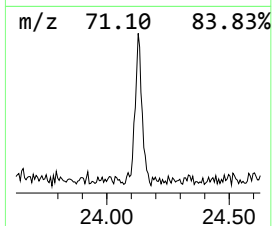
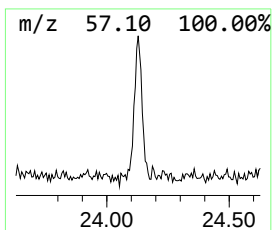
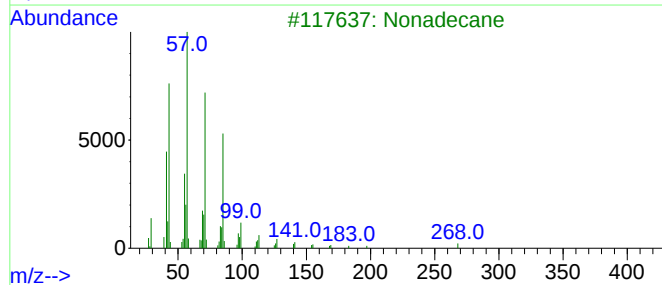
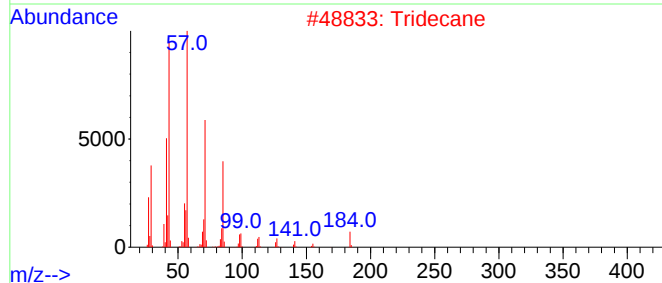
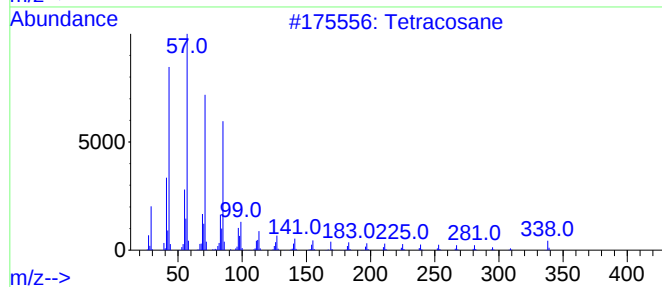
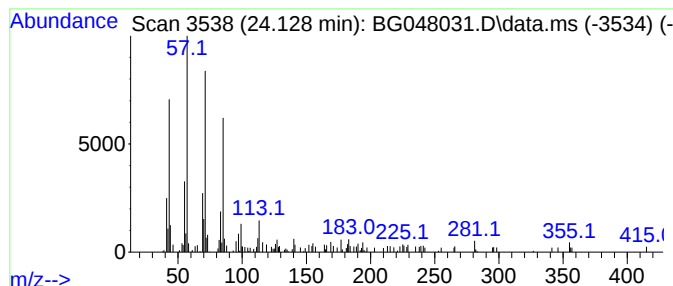
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.128	2.42 ng	111234	Perylene-d12	25.044

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	86
2			Tridecane	184	C13H28	000629-50-5	83
3			Nonadecane	268	C19H40	000629-92-5	80
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048031.D
Acq On : 27 Jan 2021 15:55
Operator : CG/JU
Sample : M1244-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB-BP24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.370	18.4	ng	847223	4	17.488	918776	20.0
unknown19.14	19.140	2.1	ng	95612	4	17.488	918776	20.0
Octadecanoic acid	19.633	11.9	ng	567567	5	21.766	957533	20.0
2,4,4,6,6,8,8-H...	20.996	5.5	ng	261376	5	21.766	957533	20.0
17-Pentatriacon...	21.402	6.2	ng	295822	5	21.766	957533	20.0
1,3-Dioxolane, ...	21.478	2.6	ng	124317	5	21.766	957533	20.0
Nonadecane	22.583	2.2	ng	104856	5	21.766	957533	20.0
Tetracosane	24.128	2.4	ng	111234	6	25.044	920522	20.0