

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
 Data File : BG060162.D
 Acq On : 23 Dec 2023 7:42
 Operator : MA/JU
 Sample : 05897-01
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-35a

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: BG060162.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.120	3	5	19	rVB	772865	1067624	10.75%	1.227%
2	5.047	326	333	338	rBV	88252	144005	1.45%	0.165%
3	5.511	404	412	427	rBV	4676297	7522217	75.73%	8.644%
4	7.103	673	683	699	rBV	4638189	8104977	81.60%	9.313%
5	7.938	818	825	833	rBV	1088103	1824979	18.37%	2.097%
6	9.101	1015	1023	1038	rBV	2878905	5054118	50.88%	5.808%
7	10.740	1294	1302	1311	rBV	1629944	2908896	29.29%	3.343%
8	13.196	1712	1720	1737	rBV	6186760	9932769	100.00%	11.414%
9	14.577	1948	1955	1962	rBV	2767867	4426999	44.57%	5.087%
10	16.063	2201	2208	2223	rBV	4740090	7081931	71.30%	8.138%
11	17.321	2413	2422	2432	rBV	3136073	4664705	46.96%	5.360%
12	18.214	2568	2574	2586	rBV2	270683	475061	4.78%	0.546%
13	19.941	2862	2868	2879	rBV	6710575	8775985	88.35%	10.084%
14	20.247	2917	2920	2927	rVB	111097	141474	1.42%	0.163%
15	21.234	3083	3088	3100	rBV2	1713664	2661688	26.80%	3.059%
16	21.586	3141	3148	3160	rVB2	2552506	4333312	43.63%	4.979%
17	21.780	3174	3181	3186	rBV2	129210	234510	2.36%	0.269%
18	22.015	3217	3221	3226	rBV4	104363	155811	1.57%	0.179%
19	22.391	3276	3285	3296	rBV4	1150913	2938402	29.58%	3.376%
20	22.667	3328	3332	3339	rVB8	87031	153513	1.55%	0.176%
21	23.255	3427	3432	3437	rVB4	66926	145233	1.46%	0.167%
22	23.402	3452	3457	3464	rBV3	189925	362766	3.65%	0.417%
23	23.860	3528	3535	3538	rBV2	361090	750485	7.56%	0.862%
24	23.913	3538	3544	3562	rVV3	1594887	3974007	40.01%	4.566%
25	24.060	3565	3569	3578	rVB3	153802	339800	3.42%	0.390%
26	24.759	3678	3688	3702	rVB3	1542434	4458034	44.88%	5.123%
27	25.305	3774	3781	3790	rVB4	159378	419786	4.23%	0.482%
28	25.911	3876	3884	3893	rVB2	277810	791257	7.97%	0.909%
29	26.028	3895	3904	3917	rBV3	653729	2213166	22.28%	2.543%
30	26.222	3932	3937	3945	rVB5	127768	332315	3.35%	0.382%
31	28.026	4238	4244	4255	rVB8	86021	305507	3.08%	0.351%
32	29.994	4571	4579	4588	rBV8	90780	329956	3.32%	0.379%

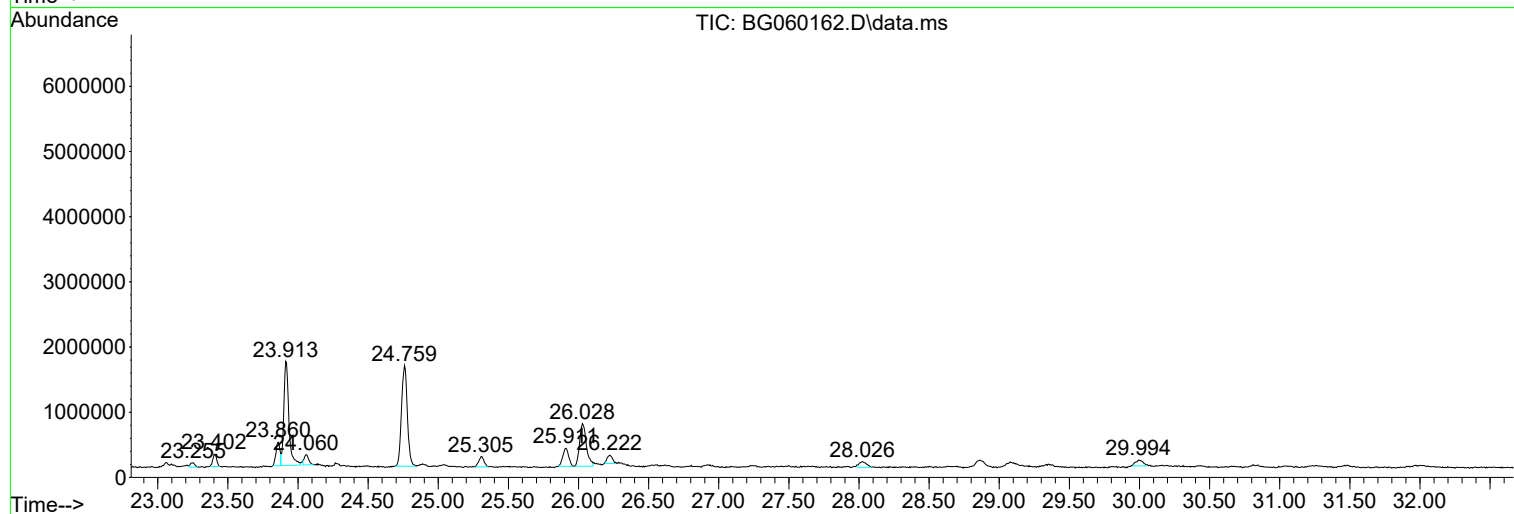
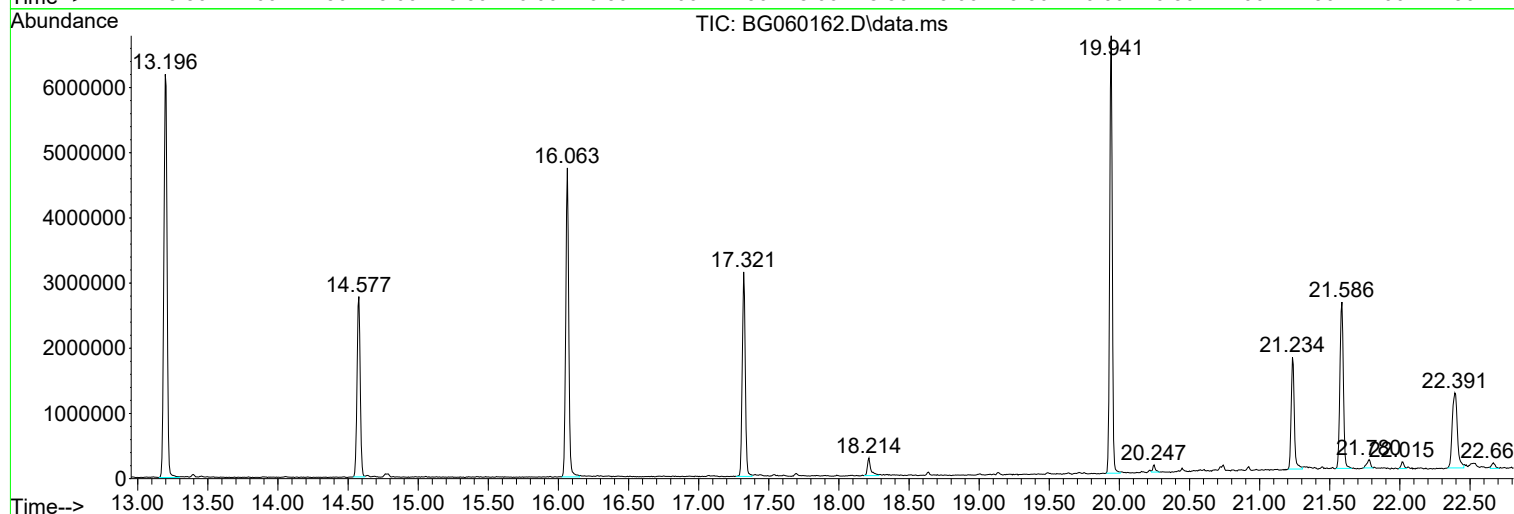
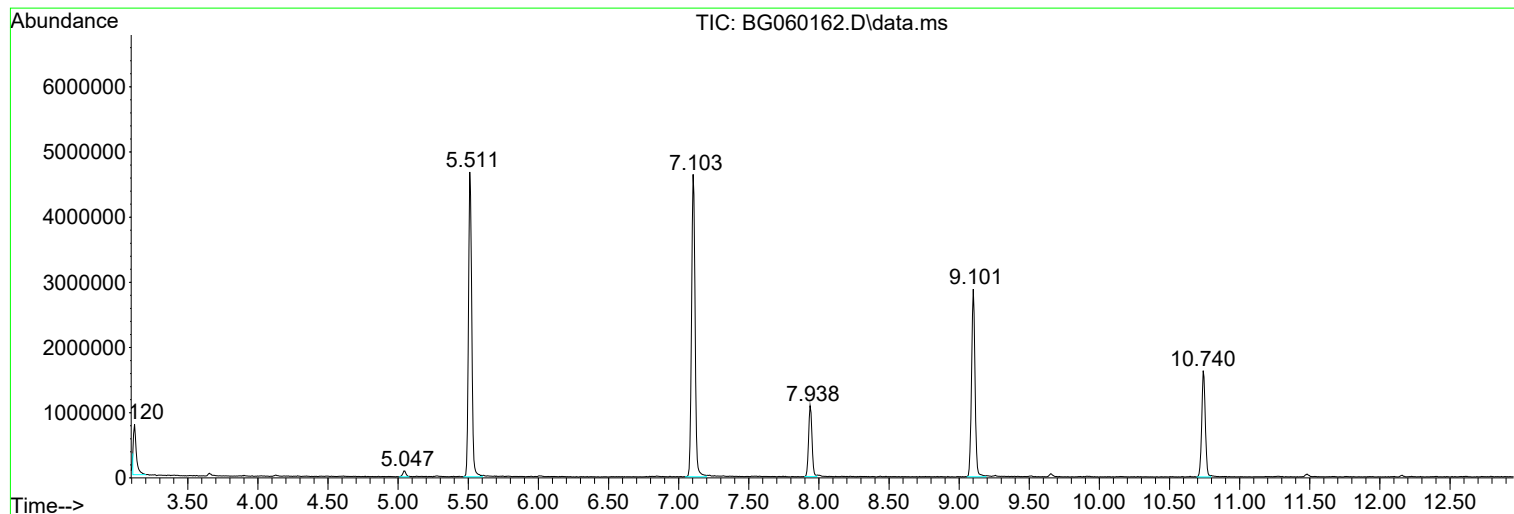
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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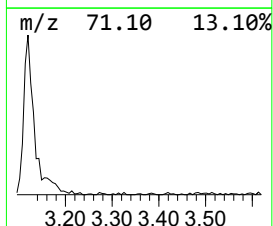
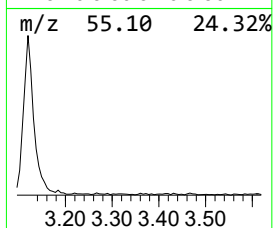
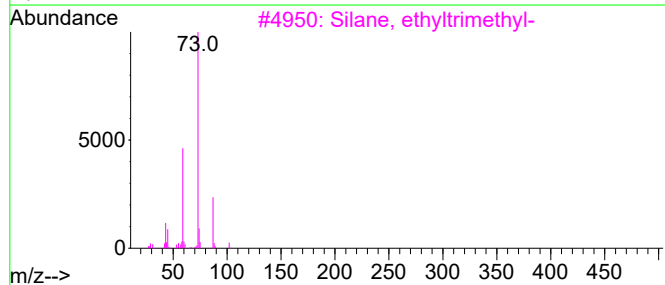
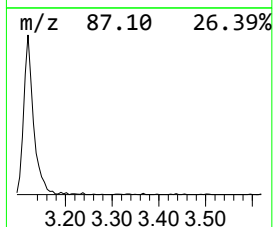
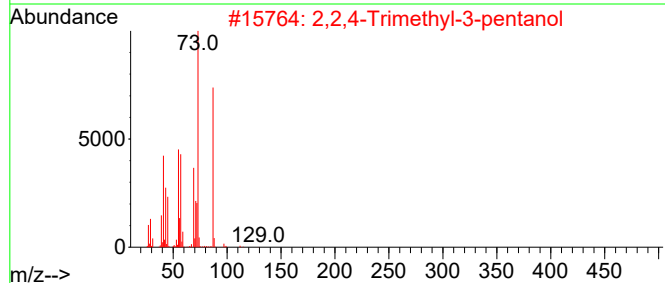
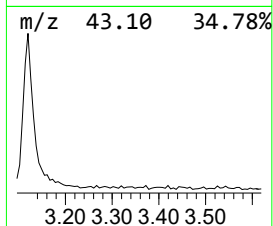
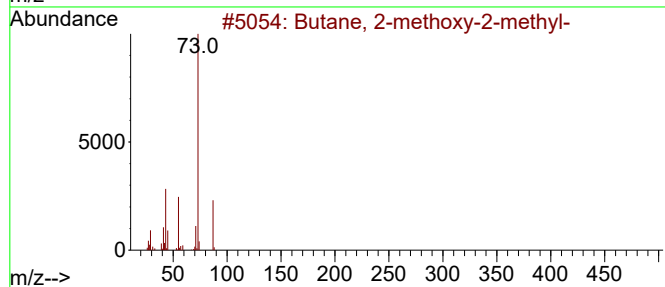
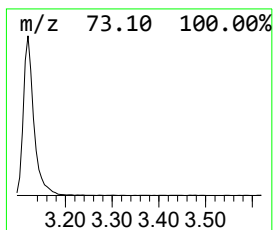
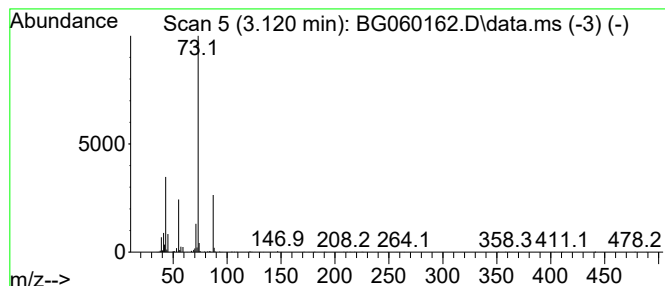
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.120	11.70 ng	1067620	1,4-Dichlorobenzene-d4	7.938

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	39
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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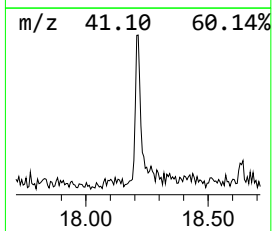
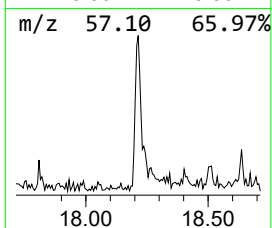
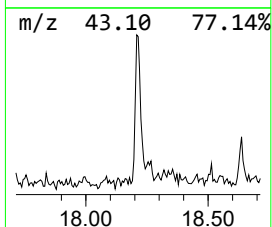
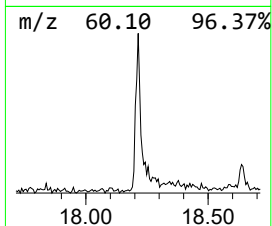
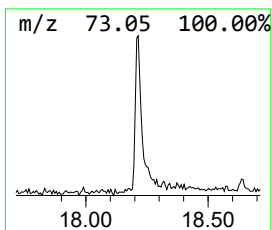
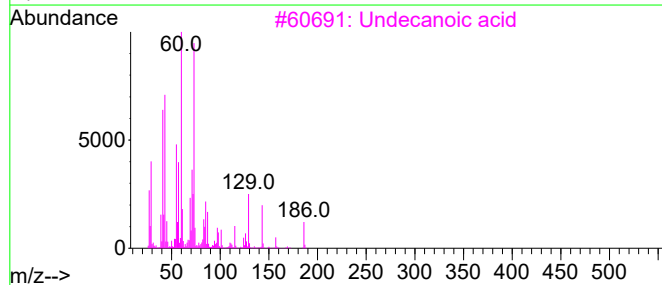
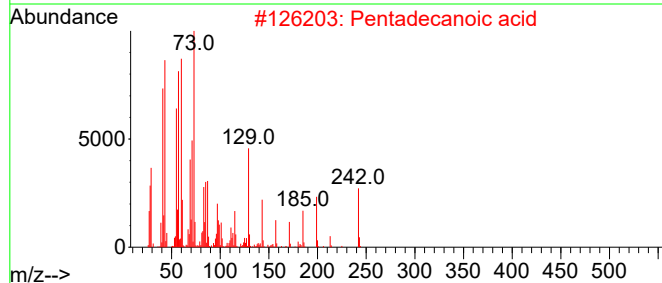
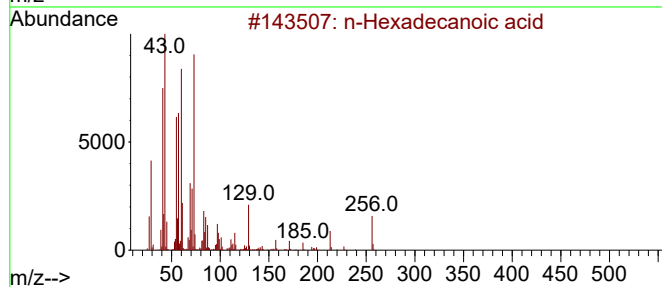
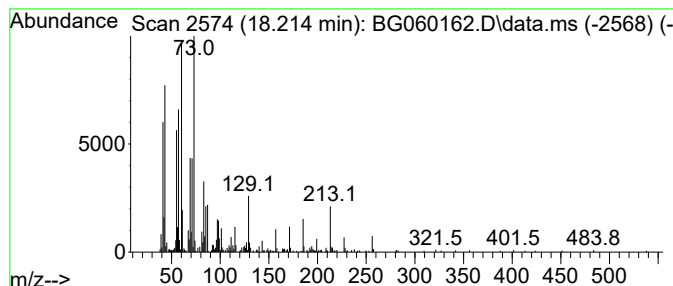
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.214	2.04 ng	475061	Phenanthrene-d10	17.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Undecanoic acid	186	C11H22O2	000112-37-8	72
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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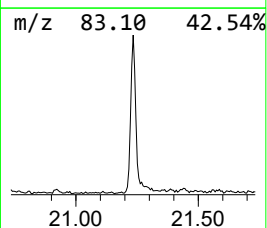
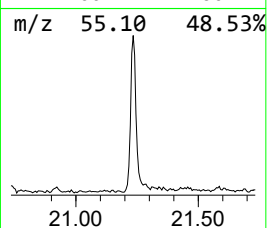
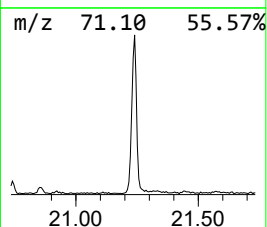
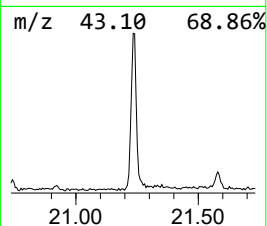
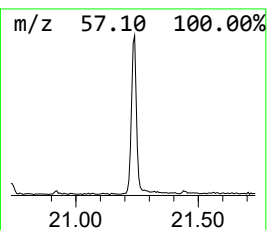
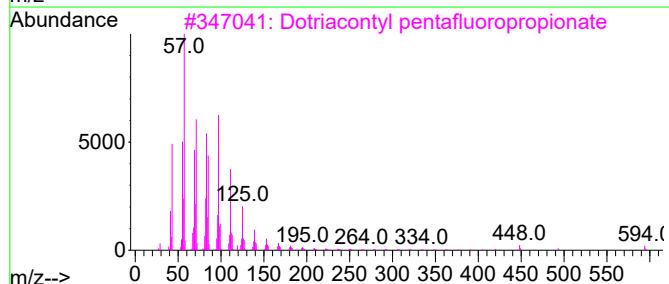
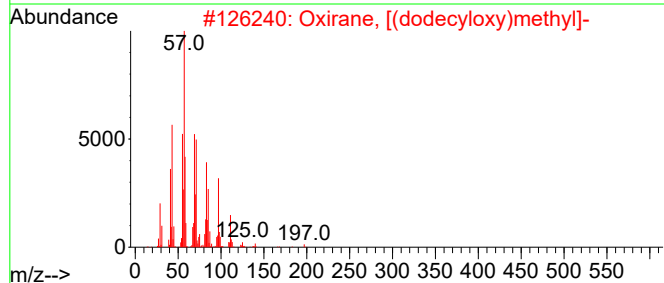
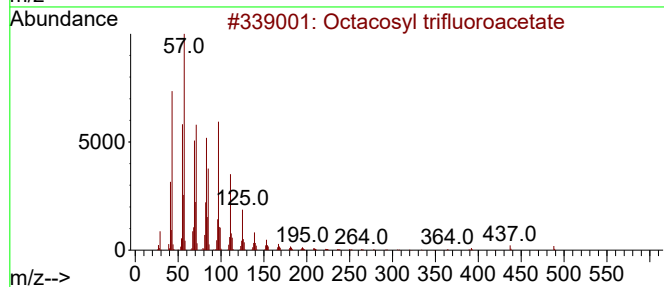
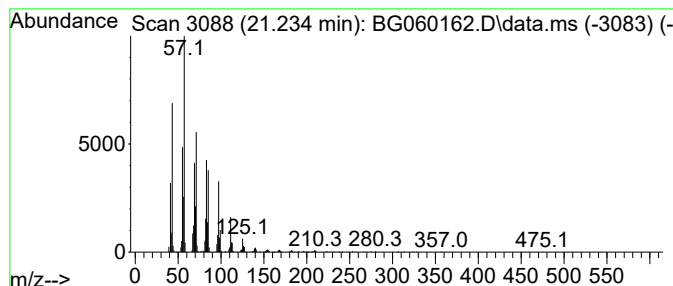
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Peak Number 3 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.234	12.28 ng	2661690	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	91
3			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
4			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
5			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	91



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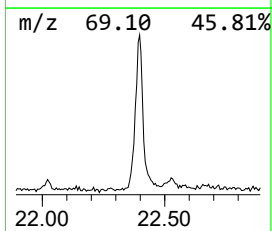
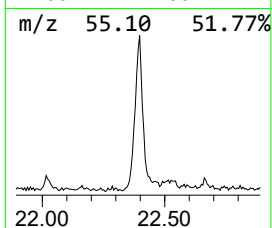
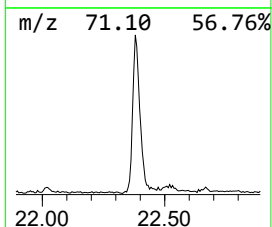
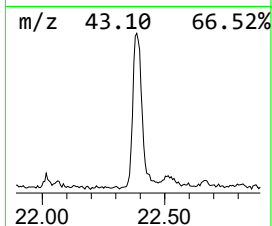
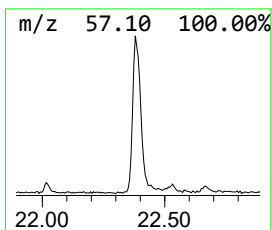
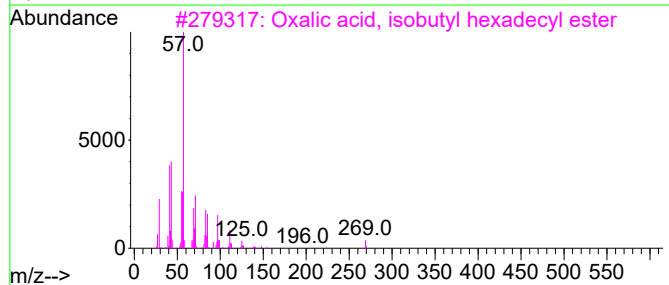
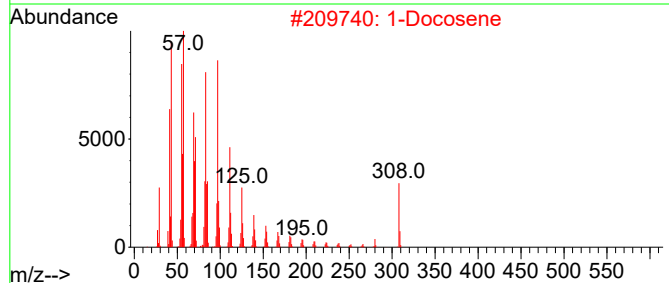
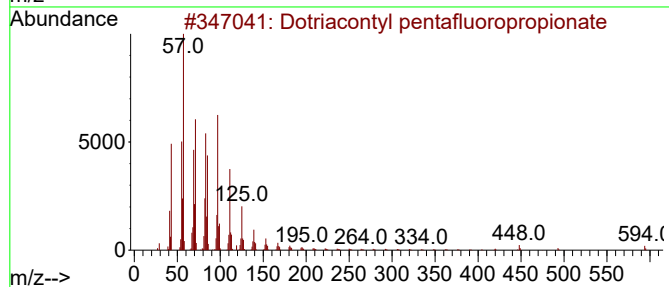
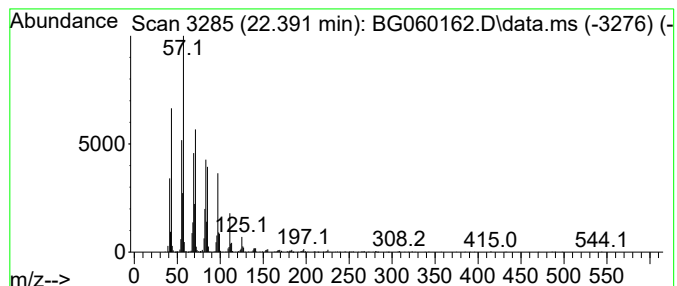
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Peak Number 4 Dotriacontyl pentafluoropro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.391	13.56 ng	2938400	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	87
2			1-Docosene	308	C22H44	001599-67-3	86
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	83
4			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	74
5			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	74



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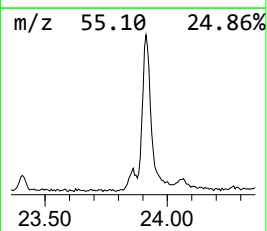
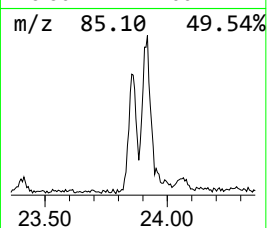
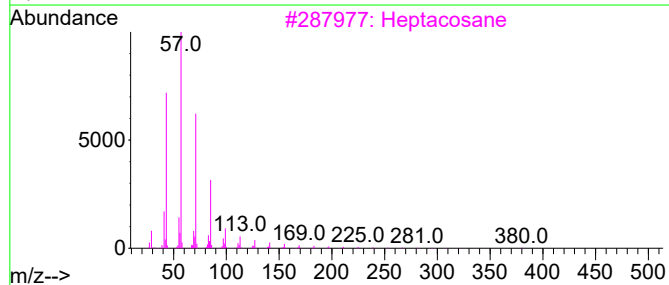
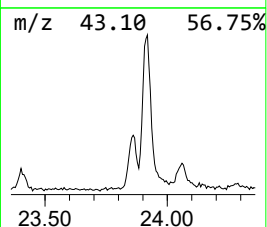
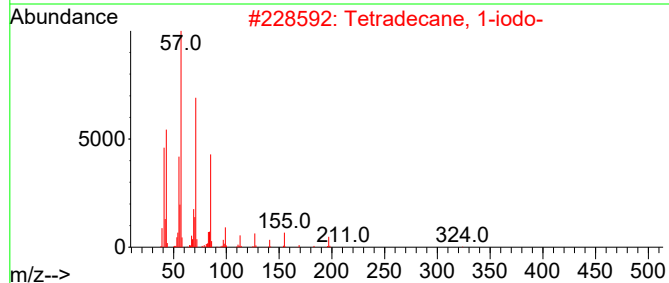
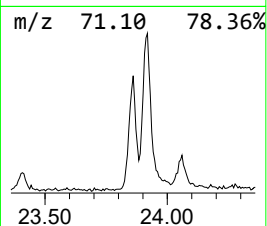
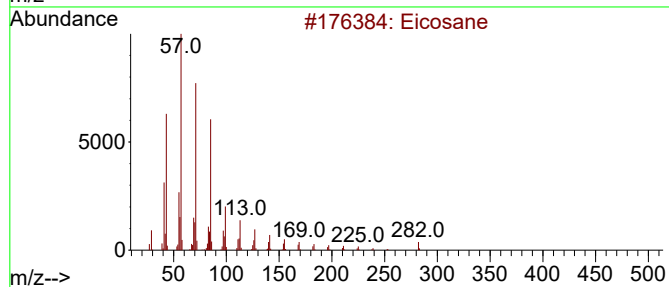
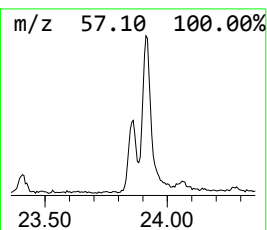
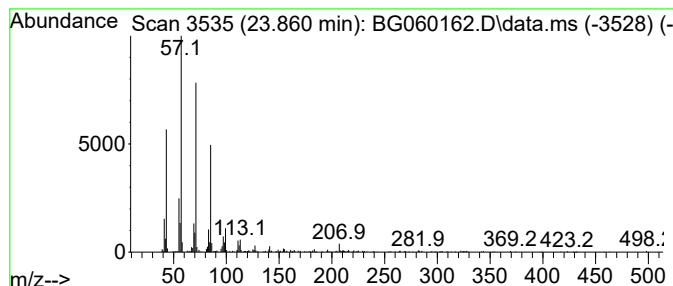
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Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.860	3.37 ng	750485	Perylene-d12	24.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	90
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
3			Heptacosane	380	C27H56	000593-49-7	72
4			Heneicosane	296	C21H44	000629-94-7	46
5			Tricosane	324	C23H48	000638-67-5	46



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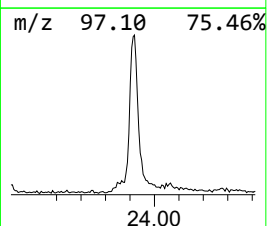
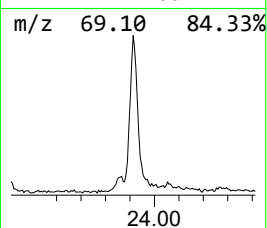
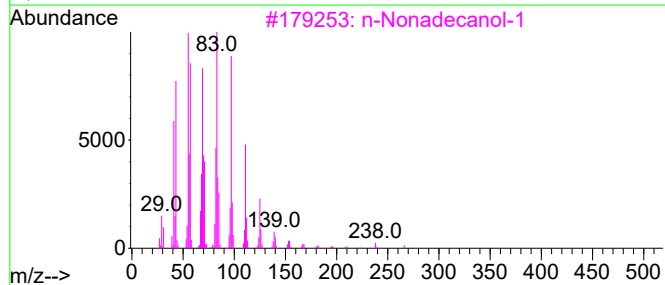
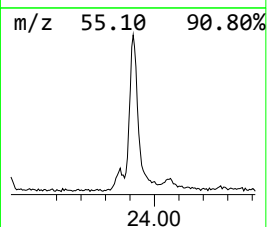
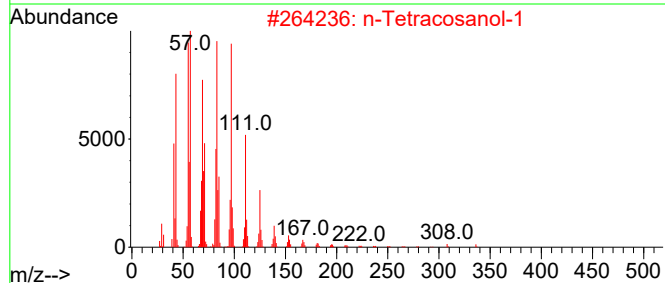
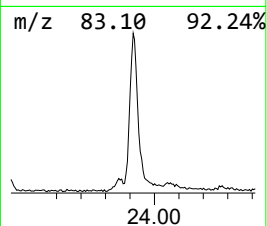
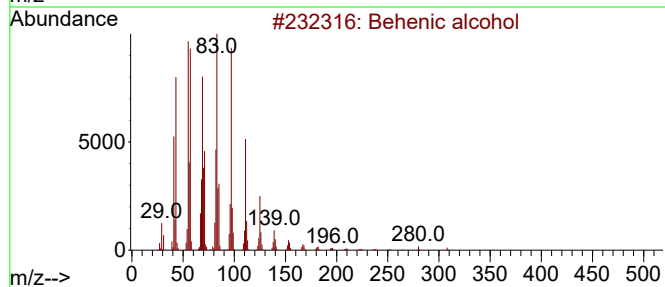
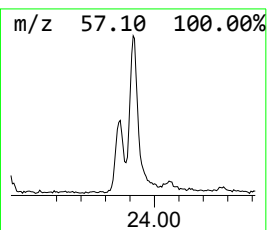
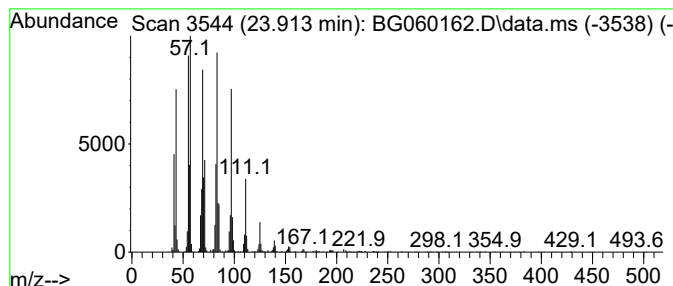
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.913	17.83 ng	3974010	Perylene-d12	24.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			Octacosanol	410	C28H58O	000557-61-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060162.D
Acq On : 23 Dec 2023 7:42
Operator : MA/JU
Sample : 05897-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-35a

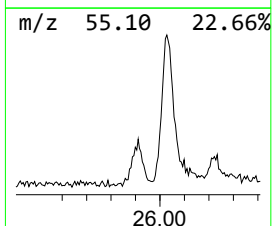
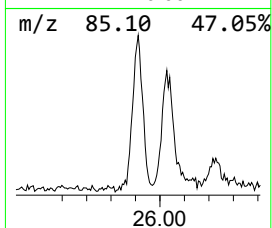
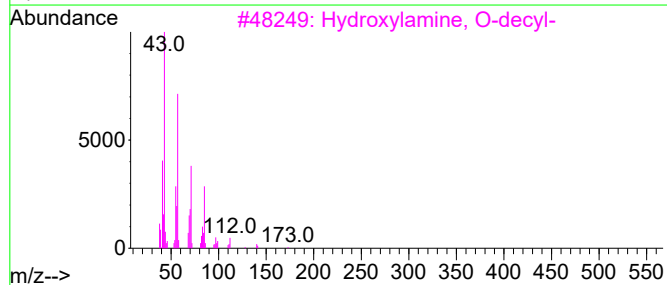
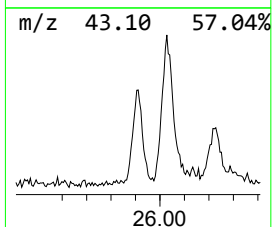
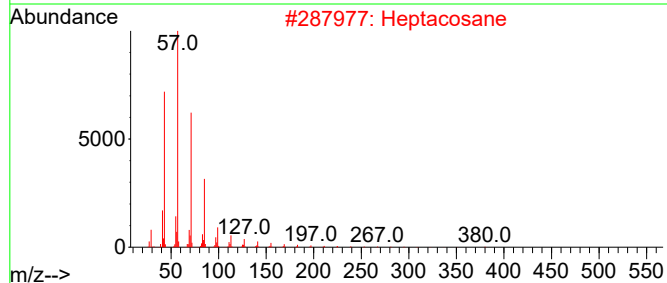
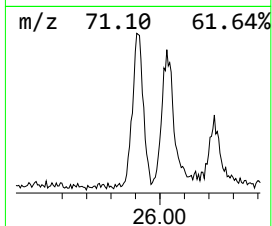
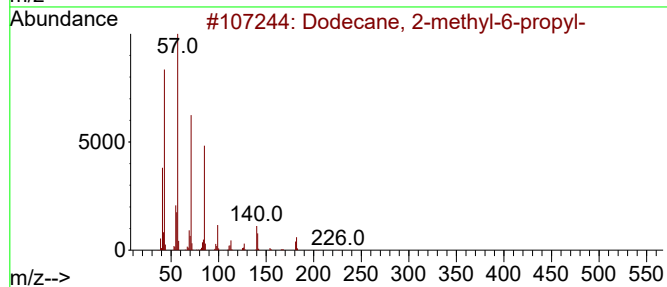
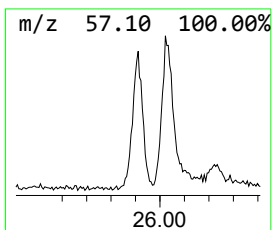
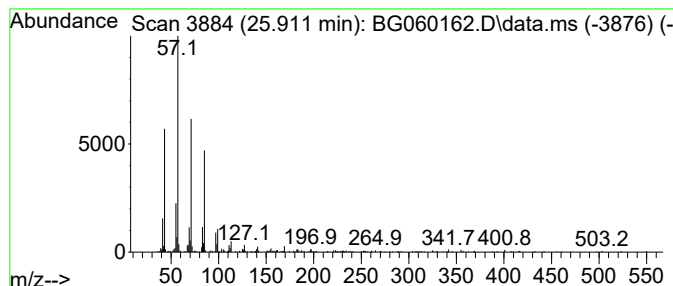
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 2-methyl-6-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.911	3.55 ng	791257	Perylene-d12	24.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	81
2			Heptacosane	380	C27H56	000593-49-7	62
3			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	59
4			Undecane, 6-ethyl-	184	C13H28	017312-60-6	49
5			Octacosane	394	C28H58	000630-02-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060162.D
Acq On : 23 Dec 2023 7:42
Operator : MA/JU
Sample : 05897-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-35a

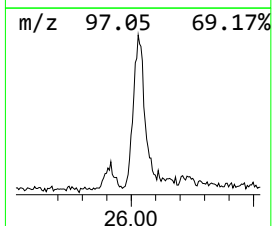
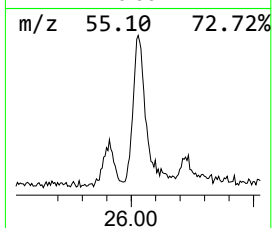
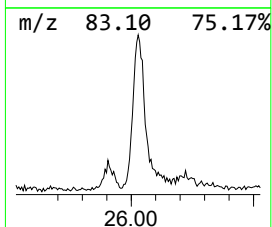
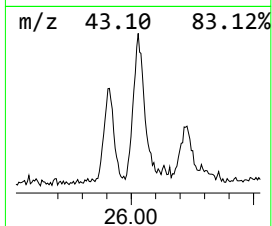
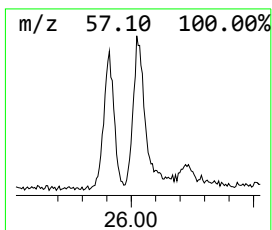
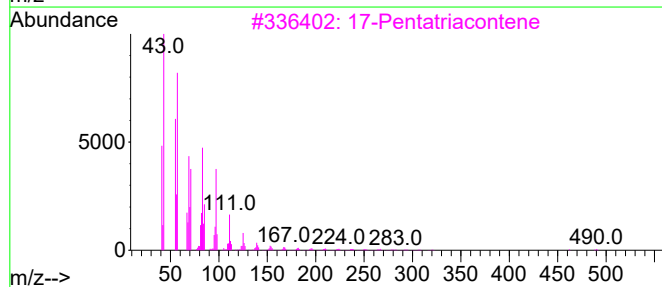
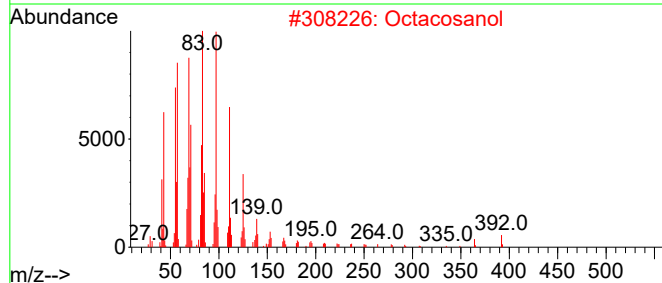
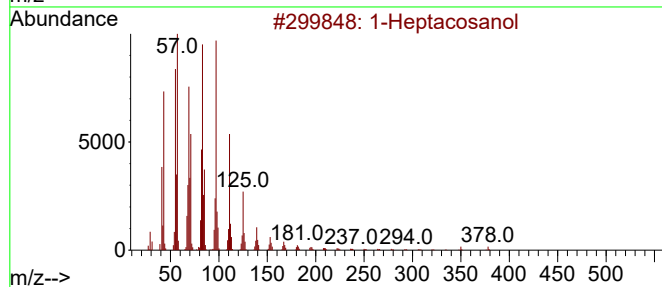
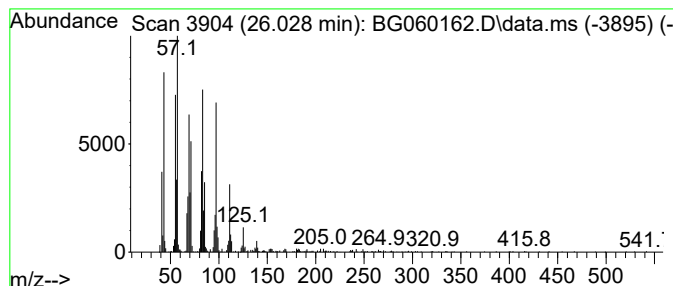
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.028	9.93 ng	2213170	Perylene-d12	24.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol			396	C27H56O	002004-39-9	94
2	Octacosanol			410	C28H58O	000557-61-9	91
3	17-Pentatriacontene			491	C35H70	006971-40-0	91
4	1-Hexacosanol			382	C26H54O	000506-52-5	91
5	1-Heneicosanol			312	C21H44O	015594-90-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060162.D
Acq On : 23 Dec 2023 7:42
Operator : MA/JU
Sample : 05897-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-35a

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...	3.120	11.7	ng	1067620	1	7.938	1824980	20.0
n-Hexadecanoic ...	18.214	2.0	ng	475061	4	17.321	4664710	20.0
Octacosyl trifl...	21.234	12.3	ng	2661690	5	21.586	4333310	20.0
Dotriacontyl pe...	22.391	13.6	ng	2938400	5	21.586	4333310	20.0
Eicosane	23.860	3.4	ng	750485	6	24.759	4458030	20.0
Behenic alcohol	23.913	17.8	ng	3974010	6	24.759	4458030	20.0
Dodecane, 2-met...	25.911	3.5	ng	791257	6	24.759	4458030	20.0
1-Heptacosanol	26.028	9.9	ng	2213170	6	24.759	4458030	20.0