

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
 Data File : BG058574.D
 Acq On : 2 Aug 2023 12:00
 Operator : MA/JU
 Sample : 03686-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-18-0-2-20230720

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-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.388	384	391	401	rBV	778454	1254073	47.33%	6.670%
2	6.986	655	663	682	rBV	779723	1328864	50.15%	7.067%
3	7.403	729	734	741	rBV2	14471	26911	1.02%	0.143%
4	7.814	795	804	809	rBV	195944	332154	12.54%	1.767%
5	7.867	809	813	821	rVB	49733	79393	3.00%	0.422%
6	8.978	994	1002	1019	rBV	450743	831306	31.37%	4.421%
7	10.611	1273	1280	1290	rBV	271054	498046	18.80%	2.649%
8	13.079	1693	1700	1718	rBV	1205913	1887219	71.22%	10.037%
9	13.672	1793	1801	1818	rBV	952047	1404911	53.02%	7.472%
10	14.459	1928	1935	1945	rBV	453280	719458	27.15%	3.826%
11	15.952	2182	2189	2209	rBV	983064	1543605	58.25%	8.209%
12	17.203	2394	2402	2415	rBV	541141	839015	31.66%	4.462%
13	18.102	2548	2555	2571	rBV2	207694	502019	18.95%	2.670%
14	19.136	2726	2731	2743	rBV	202754	303134	11.44%	1.612%
15	19.254	2744	2751	2763	rVB5	53025	123337	4.65%	0.656%
16	19.377	2767	2772	2784	rBV	184614	315474	11.91%	1.678%
17	19.824	2842	2848	2855	rBV	1920090	2649750	100.00%	14.092%
18	20.129	2895	2900	2903	rBV	44454	54128	2.04%	0.288%
19	20.617	2979	2983	2987	rBV	110626	140528	5.30%	0.747%
20	21.105	3062	3066	3069	rBV	160214	198944	7.51%	1.058%
21	21.445	3118	3124	3139	rBV	513472	949527	35.83%	5.050%
22	21.622	3150	3154	3160	rVB	212021	298268	11.26%	1.586%
23	21.939	3204	3208	3213	rBV	159667	227286	8.58%	1.209%
24	22.197	3247	3252	3257	rBV	235442	360088	13.59%	1.915%
25	22.850	3358	3363	3374	rBV	185173	343459	12.96%	1.827%
26	23.613	3487	3493	3500	rVB	163385	326760	12.33%	1.738%
27	24.512	3638	3646	3659	rBV2	419729	1265283	47.75%	6.729%

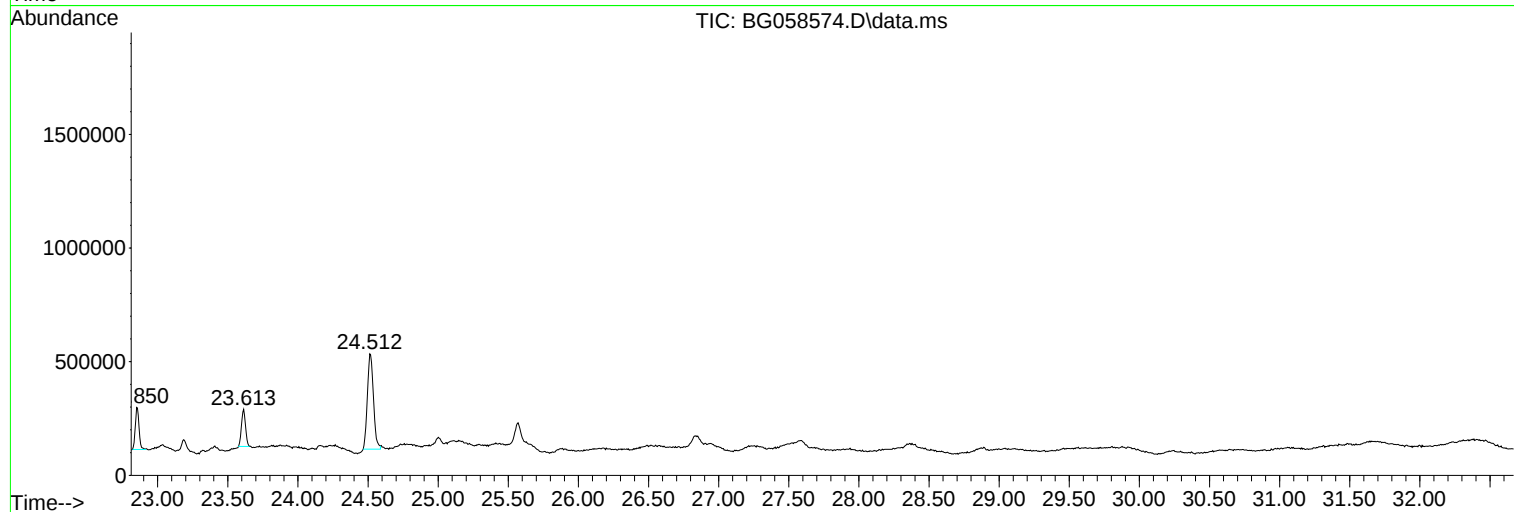
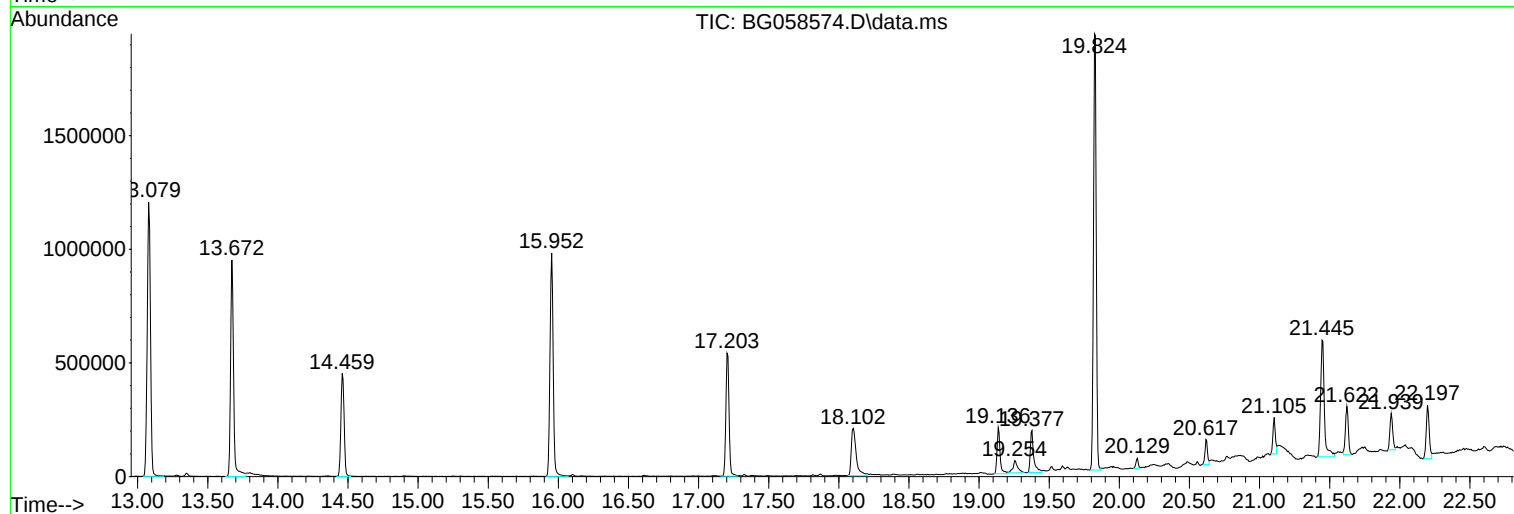
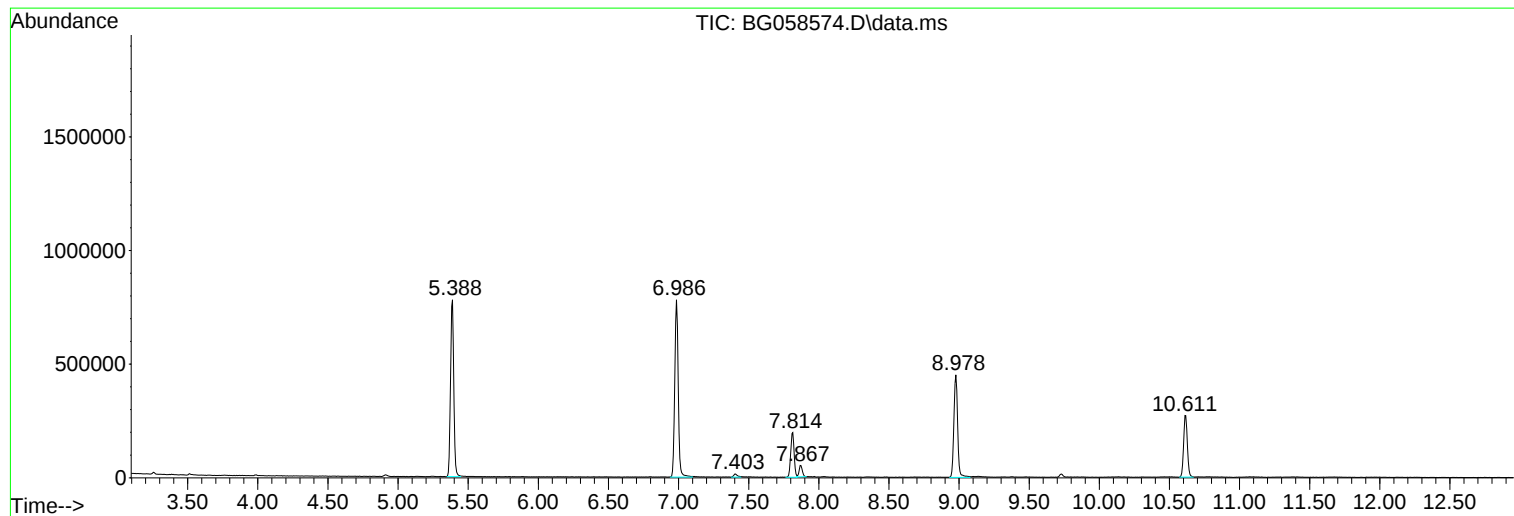
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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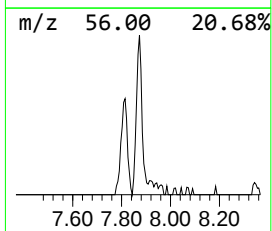
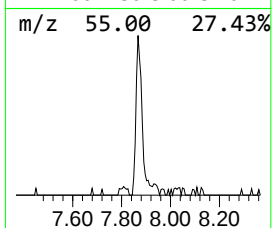
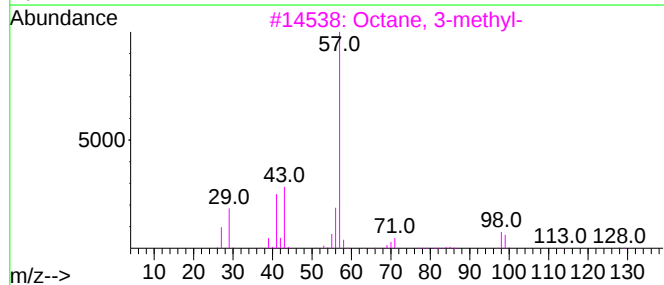
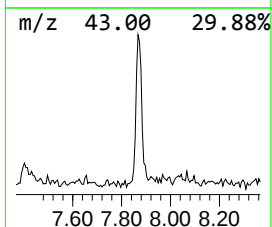
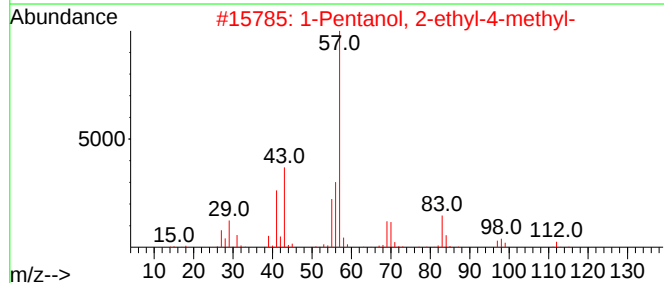
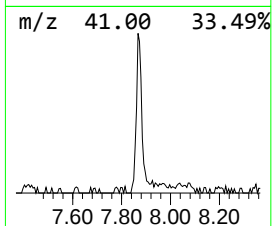
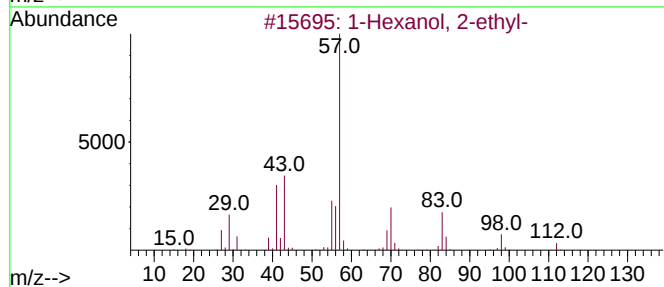
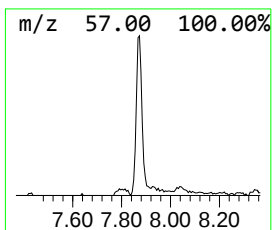
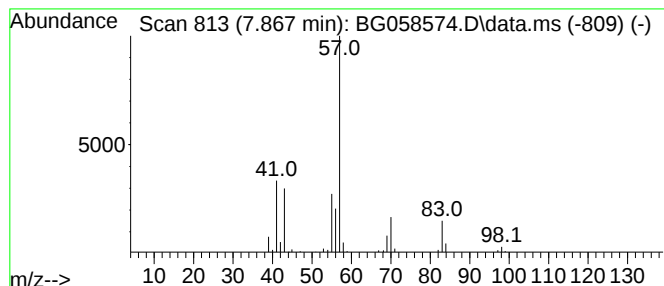
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.867	4.78 ng	79393	1,4-Dichlorobenzene-d4	7.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Octane, 3-methyl-	128	C9H20	002216-33-3	47
4			2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	42
5			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	42



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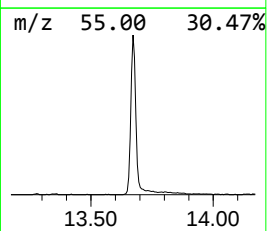
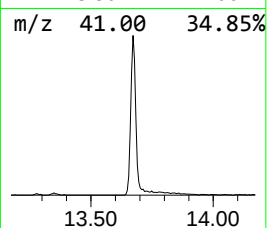
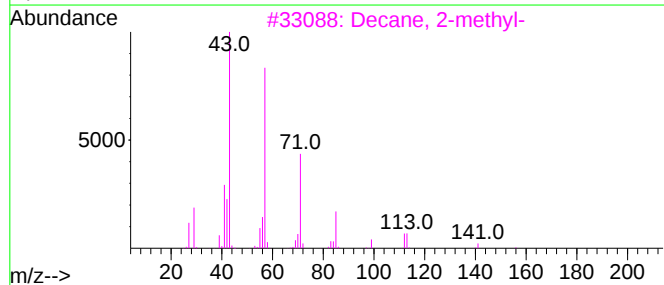
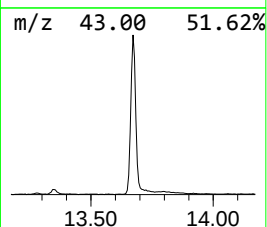
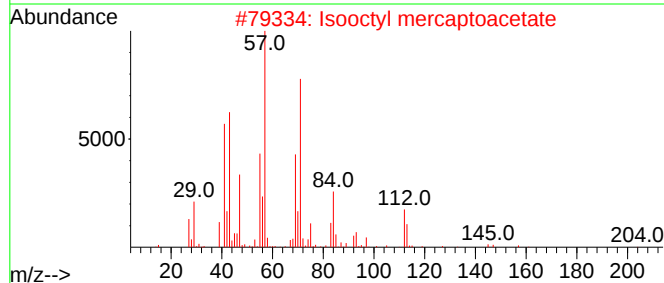
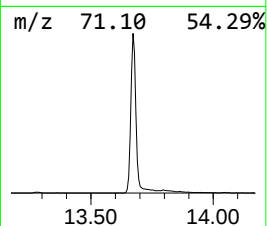
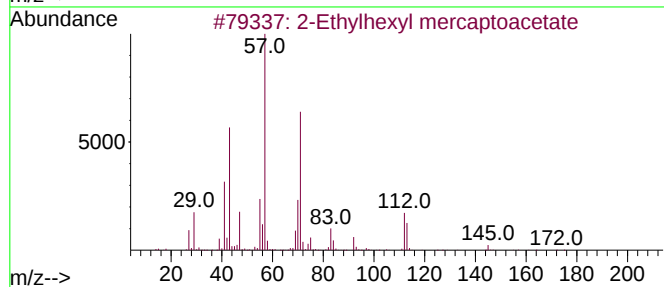
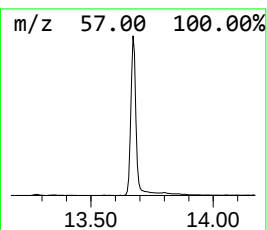
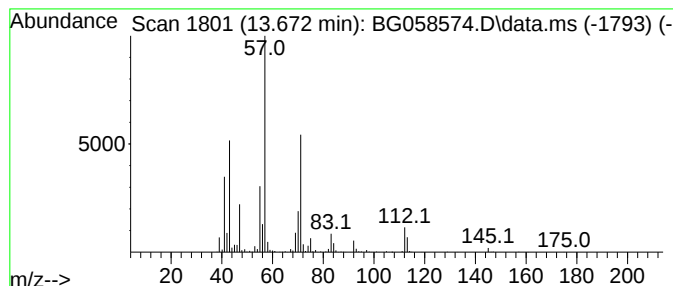
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Ethylhexyl mercaptoacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.672	39.05 ng	1404910	Acenaphthene-d10		14.459	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate		204	C10H20O2S	007659-86-1	90
2	Isooctyl mercaptoacetate		204	C10H20O2S	025103-09-7	80
3	Decane, 2-methyl-		156	C11H24	006975-98-0	53
4	Undecane, 3,6-dimethyl-		184	C13H28	017301-28-9	53
5	Dodecane, 2,6,11-trimethyl-		212	C15H32	031295-56-4	50



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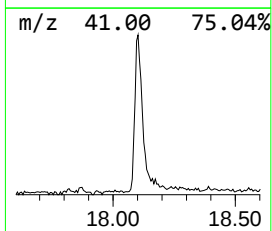
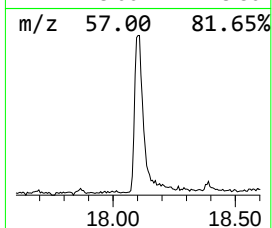
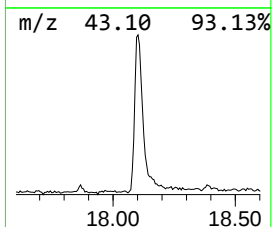
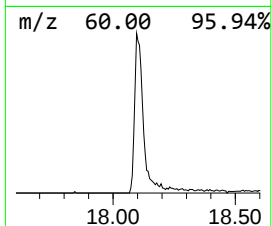
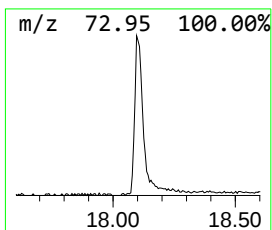
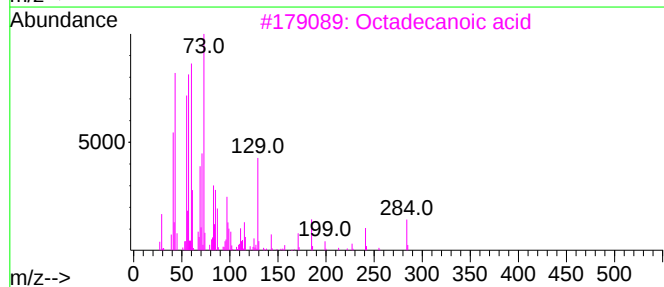
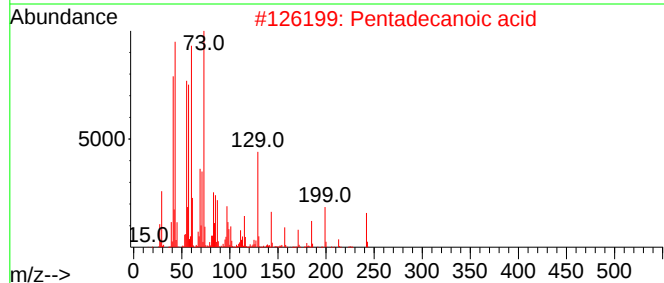
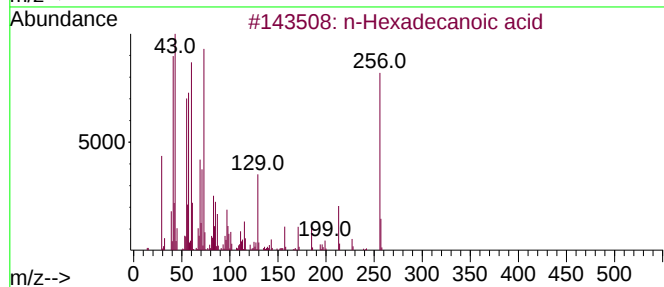
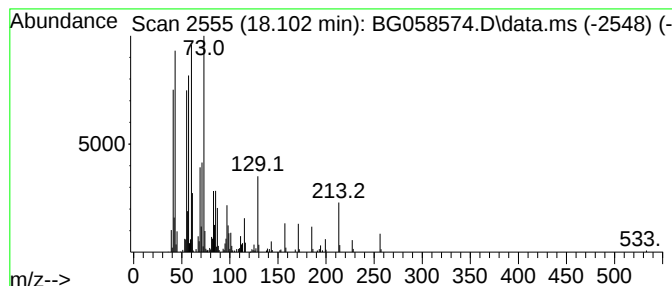
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.102	11.97 ng	502019	Phenanthrene-d10		17.203	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
3	Octadecanoic acid		284	C18H36O2	000057-11-4	76
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	74
5	Tridecanoic acid		214	C13H26O2	000638-53-9	70



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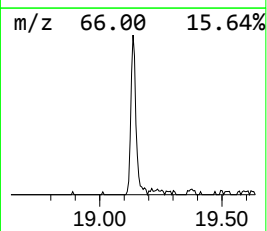
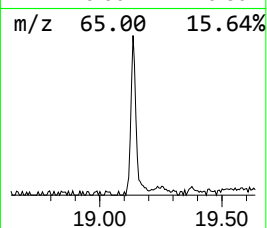
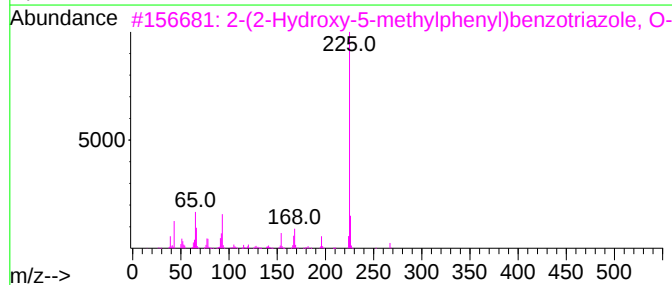
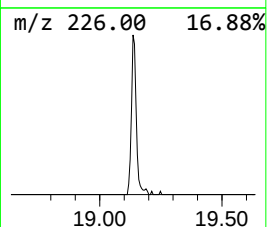
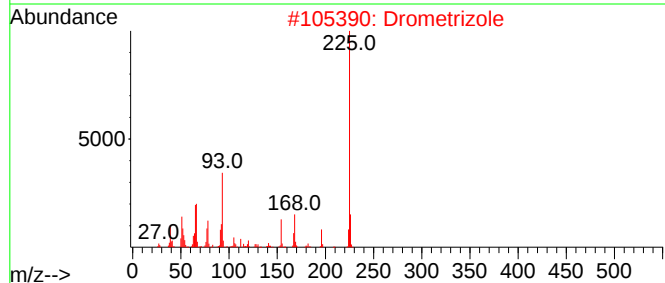
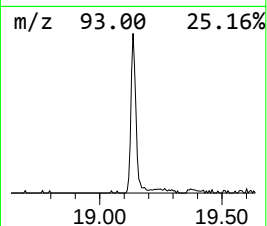
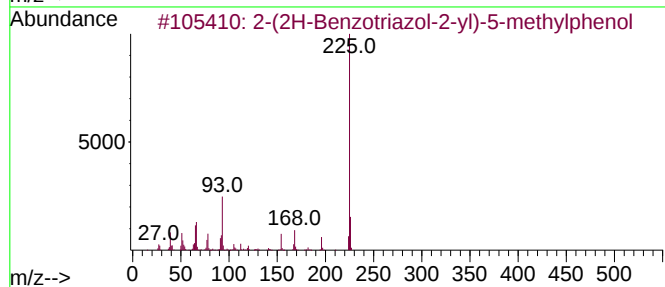
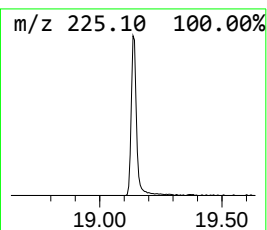
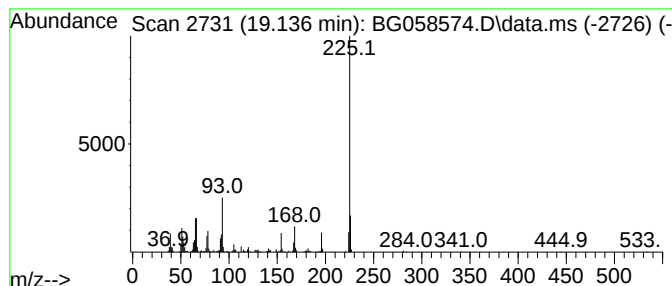
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Peak Number 4 2-(2H-Benzotriazol-2-yl)-5-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.136	7.23 ng	303134	Phenanthrene-d10	17.203

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(2H-Benzotriazol-2-yl)-5-methy...	225	C13H11N3O	004998-48-5	98
2			Drometrizole	225	C13H11N3O	002440-22-4	97
3			2-(2-Hydroxy-5-methylphenyl)benz...	267	C15H13N3O2	1000384-15-2	78
4			9(10H)-Acridinone, 1-hydroxy-10-...	225	C14H11NO2	016584-54-6	50
5			2H-Benzotriazole, 2-(2-butoxy-5-...	281	C17H19N3O	1000262-87-5	50



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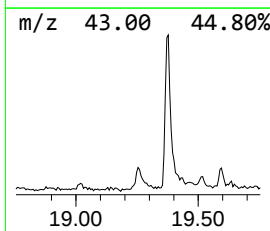
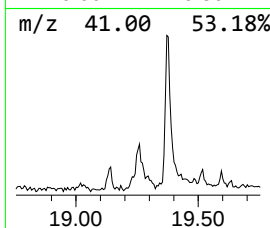
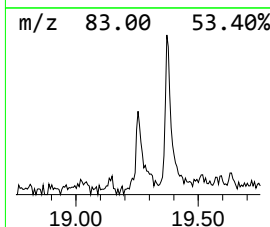
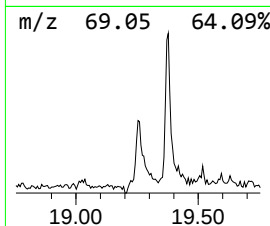
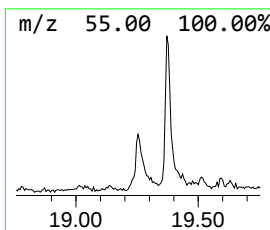
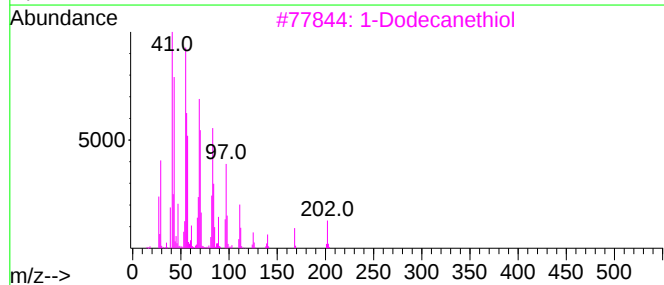
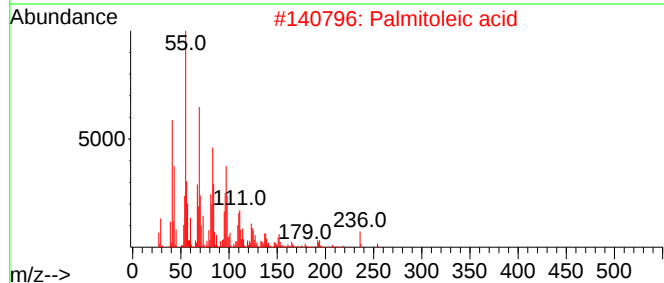
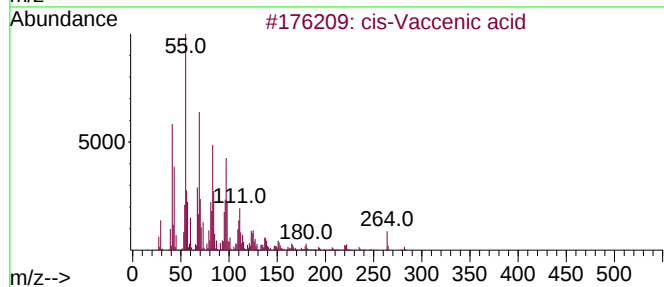
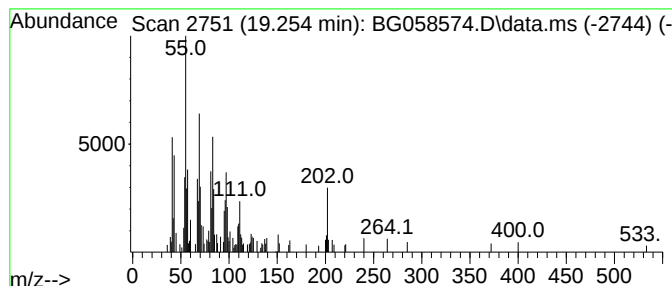
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Peak Number 5 cis-Vaccenic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.254	2.94 ng	123337	Phenanthrene-d10	17.203

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
2			Palmitoleic acid	254	C16H30O2	000373-49-9	81
3			1-Dodecanethiol	202	C12H26S	000112-55-0	76
4			Oxacyclohexadecan-2-one	240	C15H28O2	000106-02-5	76
5			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	74



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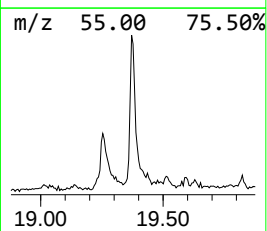
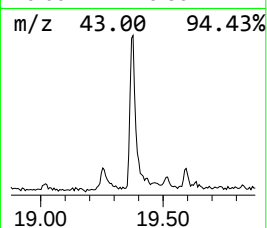
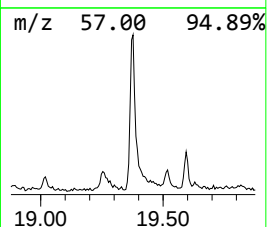
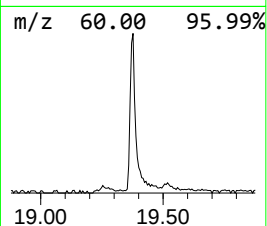
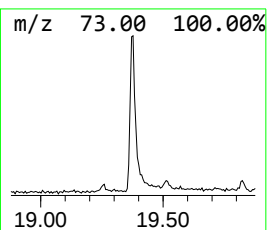
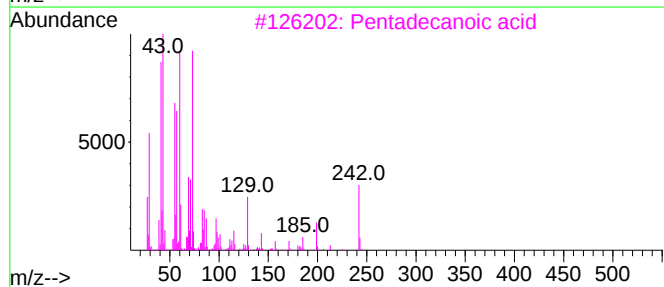
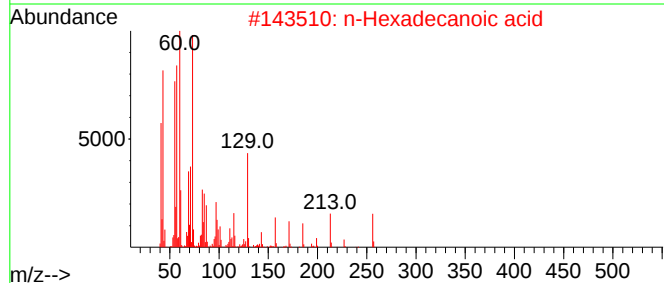
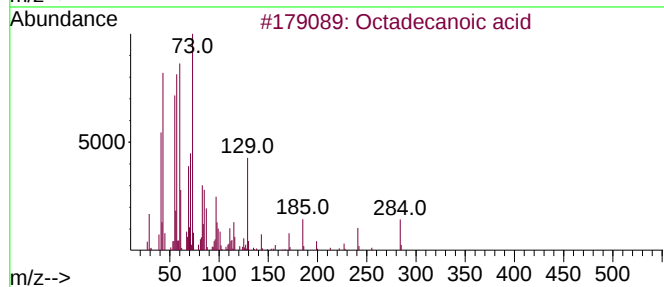
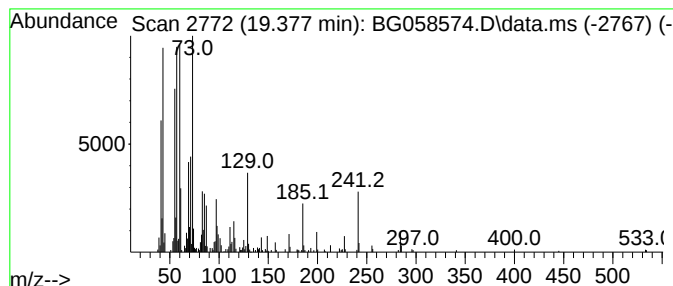
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.377	6.64 ng	315474	Chrysene-d12	21.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058574.D
Acq On : 2 Aug 2023 12:00
Operator : MA/JU
Sample : 03686-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

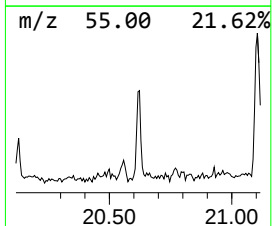
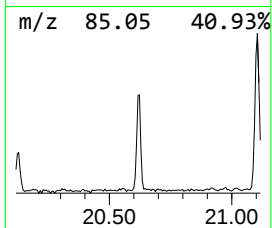
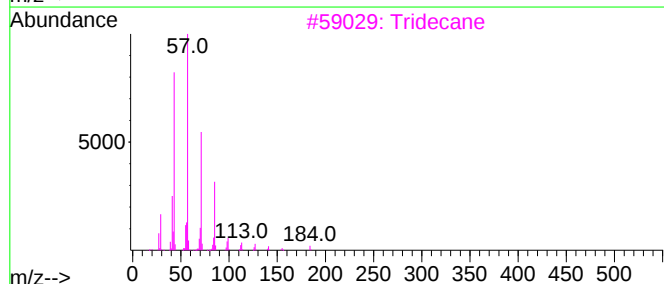
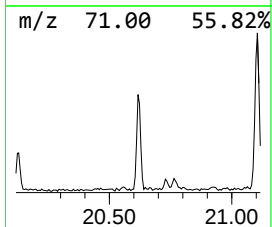
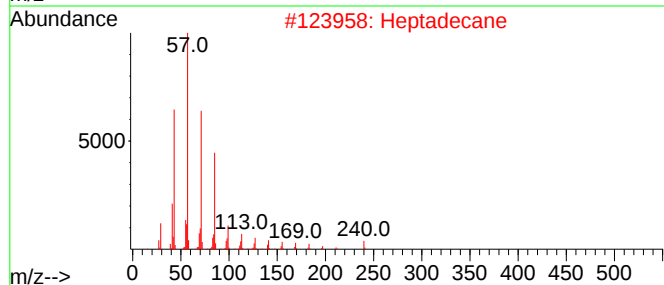
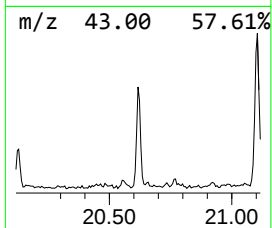
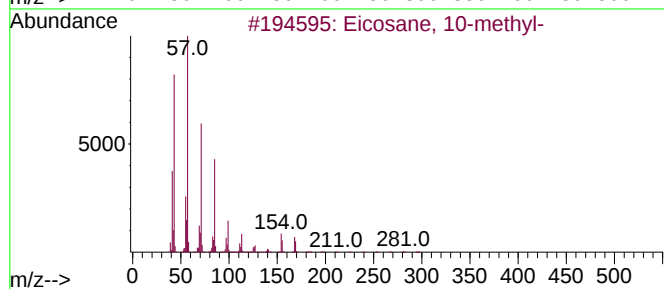
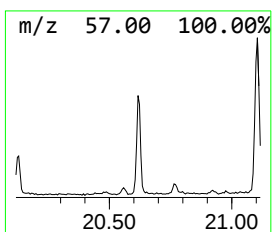
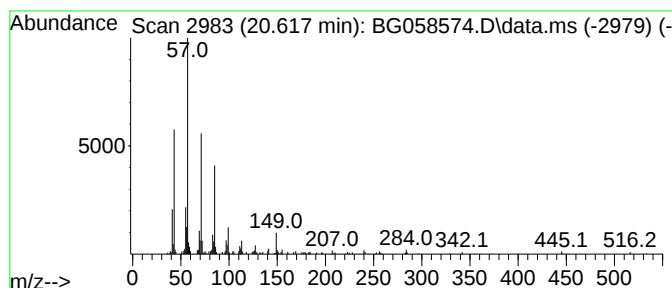
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ClientSampleId :
SB-18-0-2-20230720

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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 Eicosane, 10-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.617	2.96 ng	140528	Chrysene-d12	21.445	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
2	Heptadecane	240	C17H36	000629-78-7	87
3	Tridecane	184	C13H28	000629-50-5	81
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	81
5	Heptacosane	380	C27H56	000593-49-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058574.D
Acq On : 2 Aug 2023 12:00
Operator : MA/JU
Sample : 03686-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-18-0-2-20230720

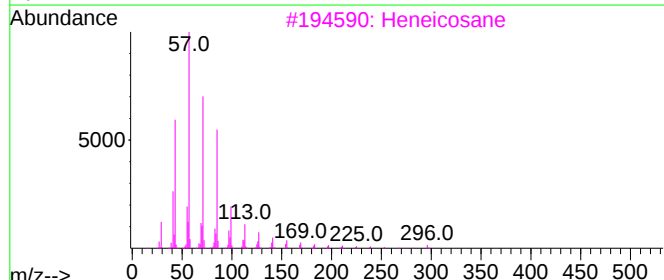
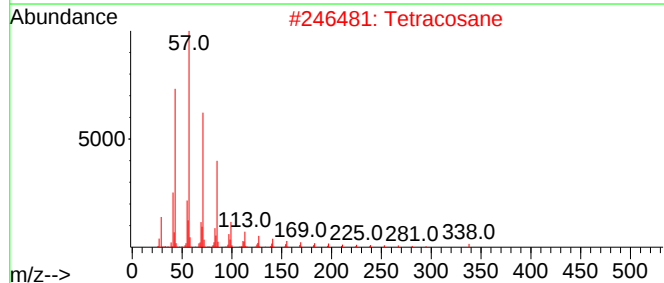
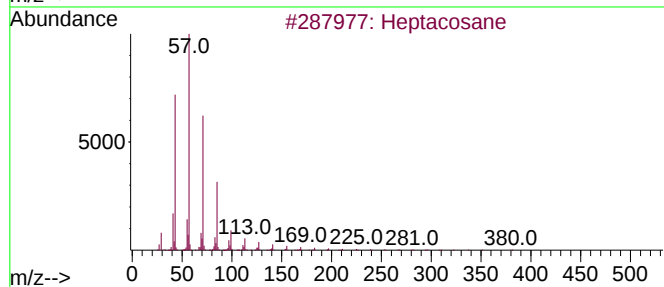
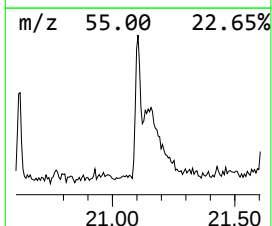
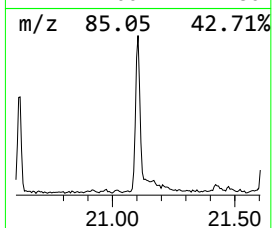
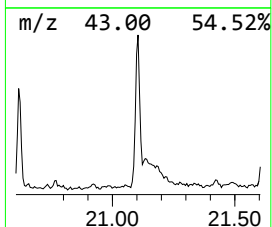
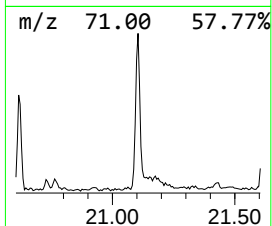
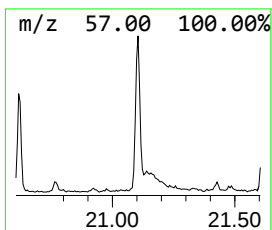
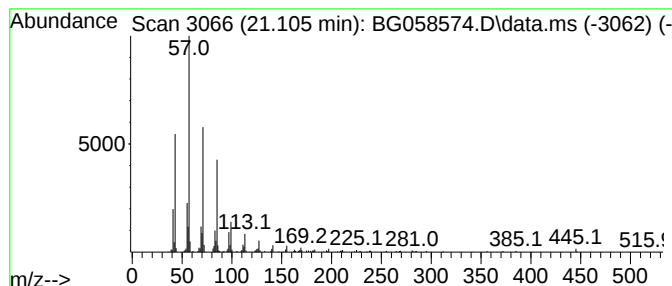
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.105	4.19 ng	198944	Chrysene-d12	21.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Heneicosane	296	C21H44	000629-94-7	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058574.D
Acq On : 2 Aug 2023 12:00
Operator : MA/JU
Sample : 03686-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-18-0-2-20230720

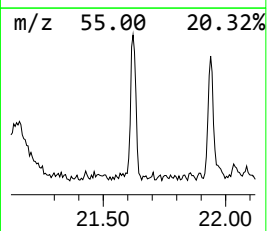
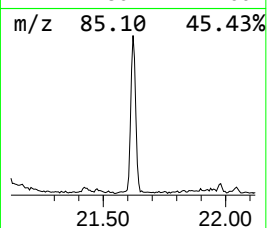
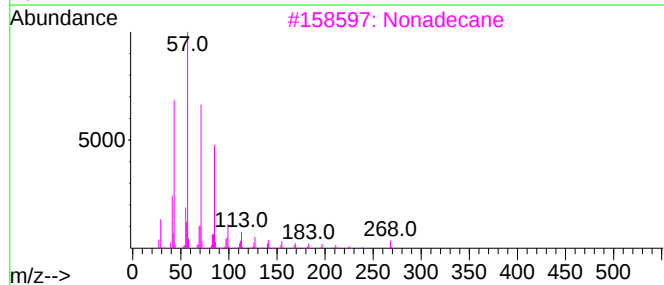
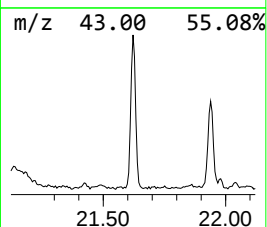
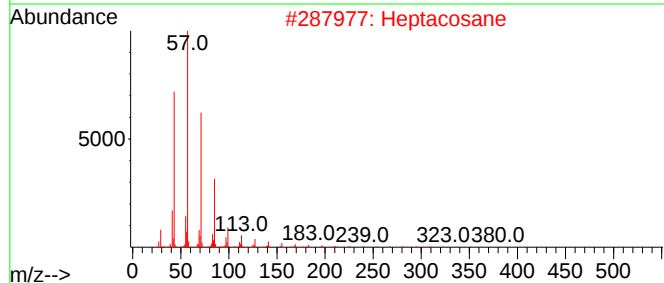
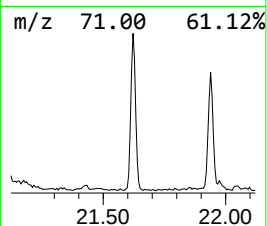
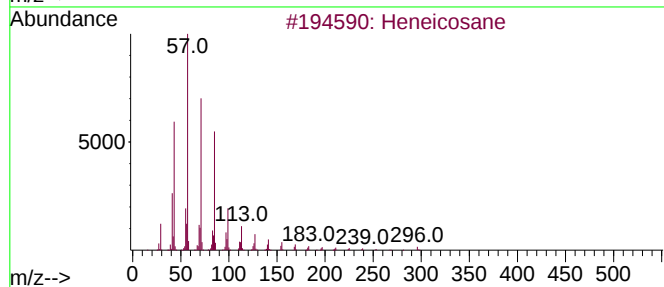
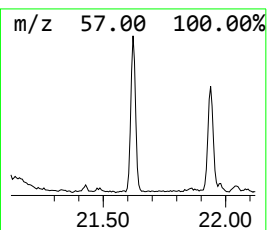
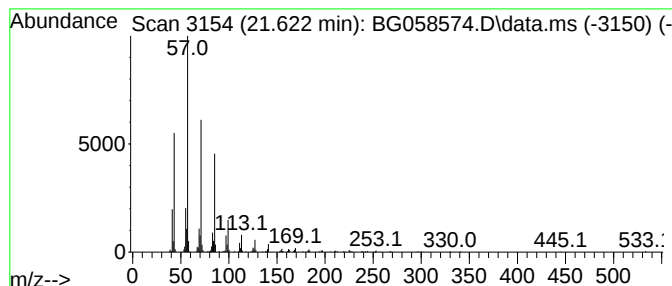
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.622	6.28 ng	298268	Chrysene-d12	21.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Nonadecane	268	C19H40	000629-92-5	90
4			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	90
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058574.D
Acq On : 2 Aug 2023 12:00
Operator : MA/JU
Sample : 03686-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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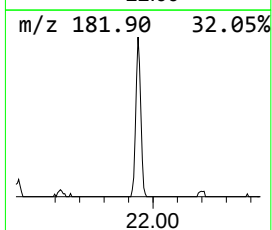
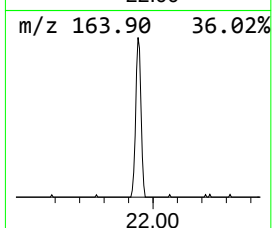
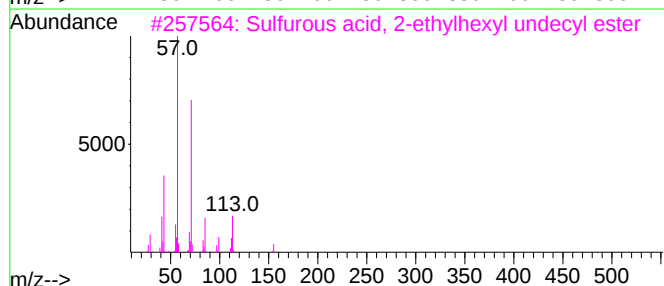
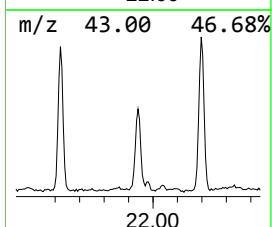
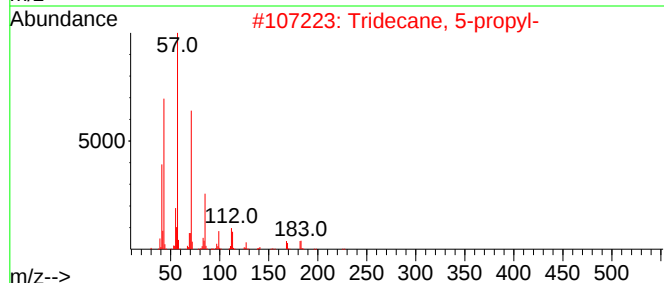
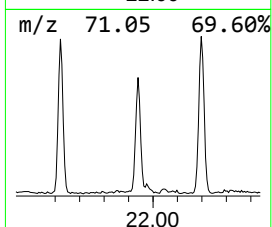
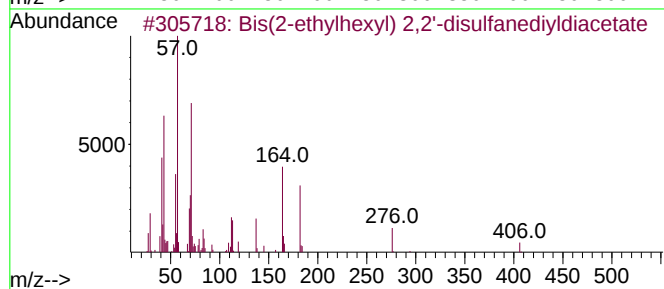
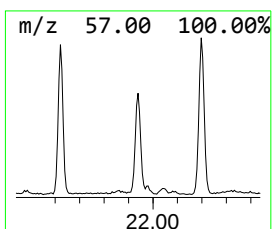
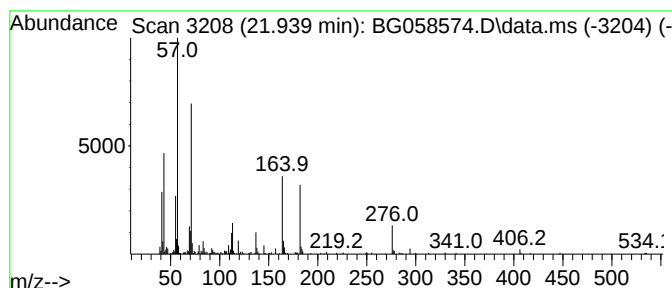
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Bis(2-ethylhexyl) 2,2'-disu... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.939	4.79 ng	227286	Chrysene-d12	21.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) 2,2'-disulfane...	406	C20H38O4S2	062268-47-7	55
2			Tridecane, 5-propyl-	226	C16H34	055045-11-9	43
3			Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	38
4			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	38
5			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058574.D
Acq On : 2 Aug 2023 12:00
Operator : MA/JU
Sample : 03686-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-18-0-2-20230720

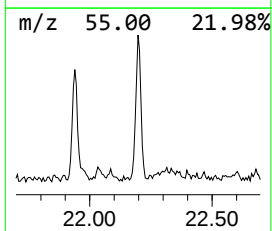
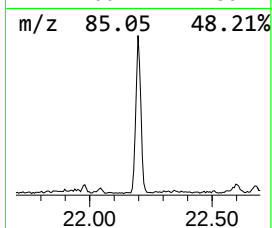
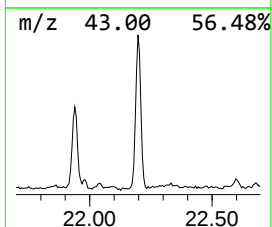
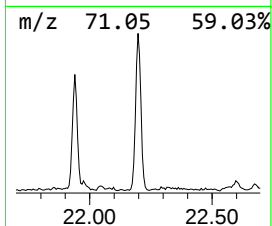
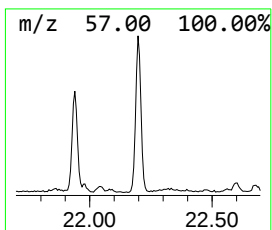
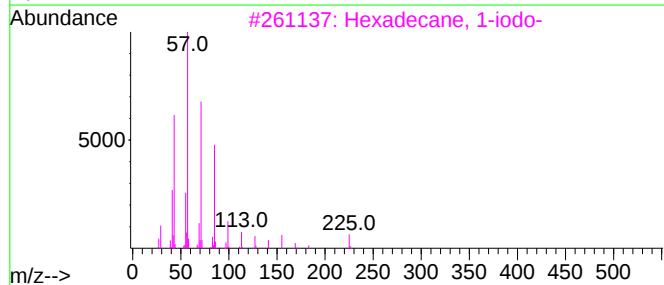
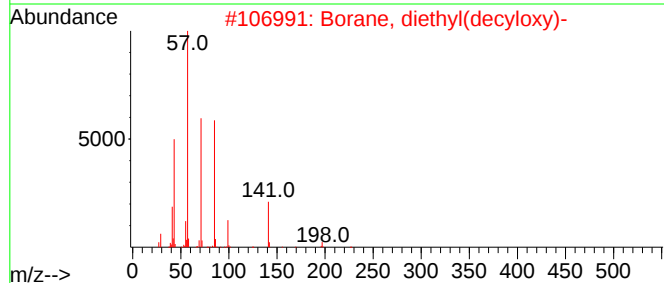
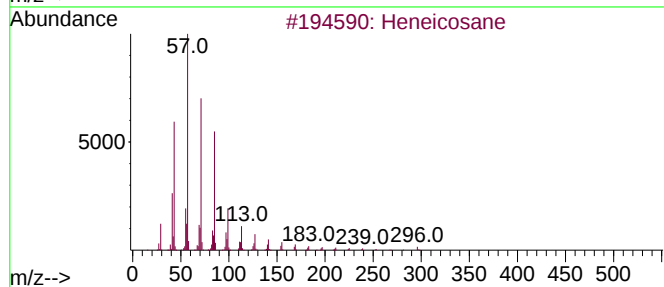
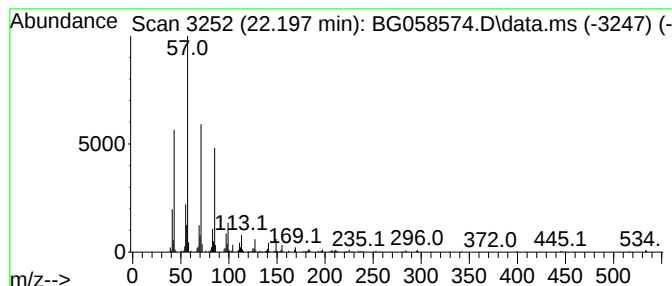
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Borane, diethyl(decyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.197	7.58 ng	360088	Chrysene-d12	21.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	98
2		Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	87
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
4		Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	83
5		Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058574.D
Acq On : 2 Aug 2023 12:00
Operator : MA/JU
Sample : 03686-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-18-0-2-20230720

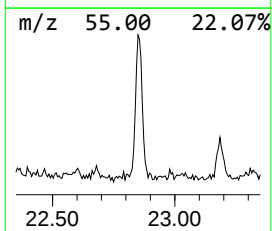
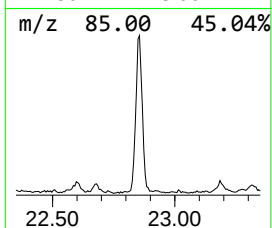
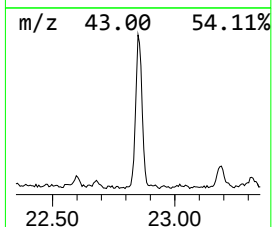
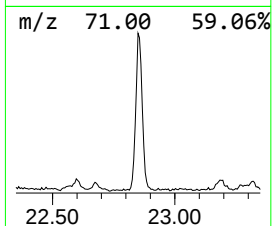
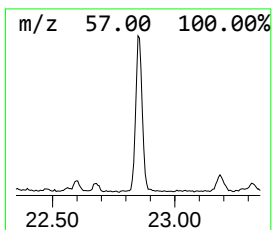
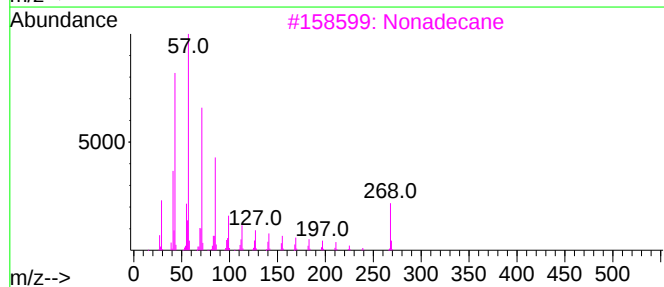
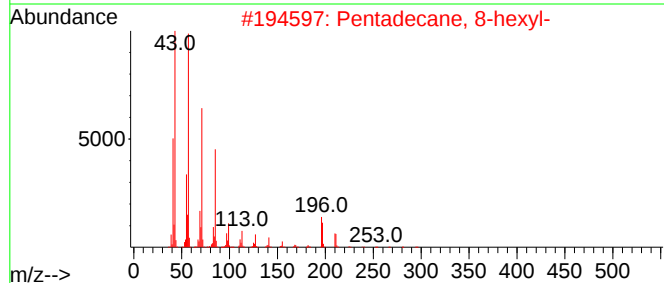
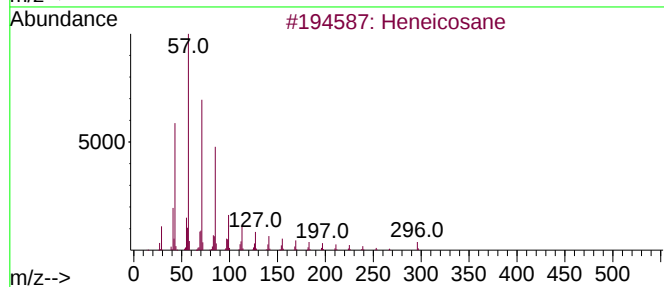
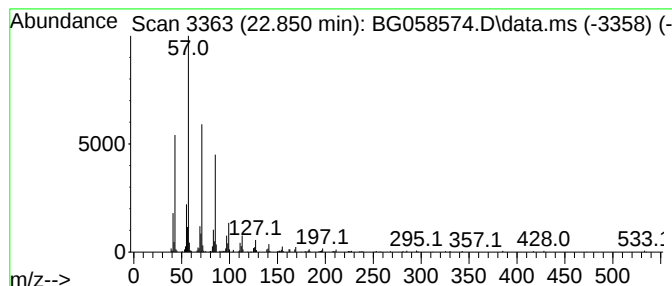
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentadecane, 8-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.849	7.23 ng	343459	Chrysene-d12	21.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	95
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
3		Nonadecane	268	C19H40	000629-92-5	89
4		Tridecane, 7-propyl-	226	C16H34	055045-09-5	87
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058574.D
Acq On : 2 Aug 2023 12:00
Operator : MA/JU
Sample : 03686-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-18-0-2-20230720

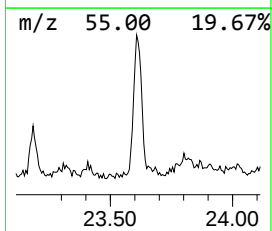
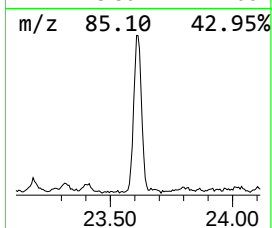
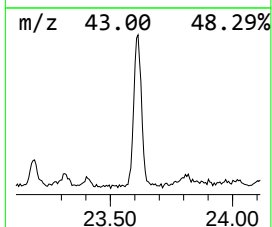
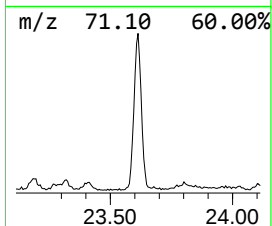
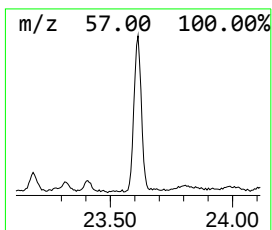
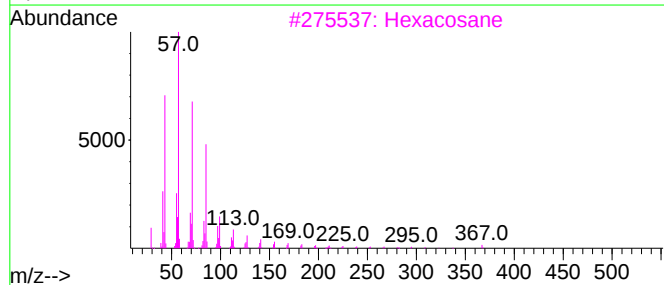
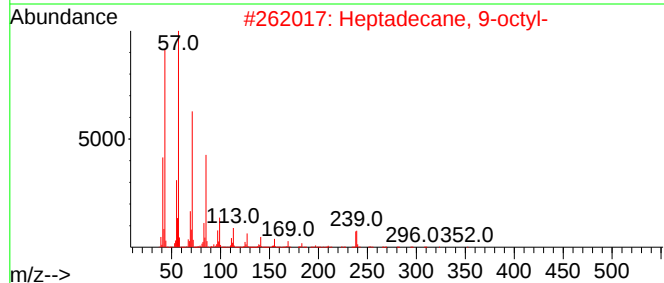
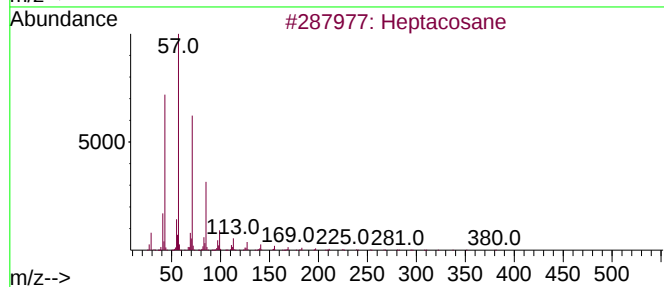
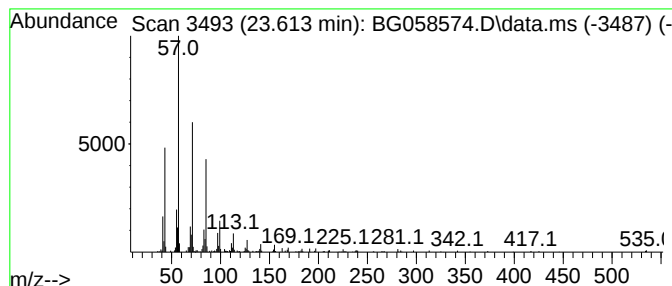
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.613	5.17 ng	326760	Perylene-d12	24.518

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	90
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Octadecane	254	C18H38	000593-45-3	87
5		Eicosane, 2-methyl-	296	C21H44	001560-84-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058574.D
Acq On : 2 Aug 2023 12:00
Operator : MA/JU
Sample : 03686-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-18-0-2-20230720

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
1-Hexanol, 2-et...	7.867	4.8	ng	79393	1	7.814	332154	20.0
2-Ethylhexyl me...	13.672	39.0	ng	1404910	3	14.459	719458	20.0
n-Hexadecanoic ...	18.102	12.0	ng	502019	4	17.203	839015	20.0
2-(2H-Benzotria...	19.136	7.2	ng	303134	4	17.203	839015	20.0
cis-Vaccenic acid	19.254	2.9	ng	123337	4	17.203	839015	20.0
Octadecanoic acid	19.377	6.6	ng	315474	5	21.445	949527	20.0
Eicosane, 10-me...	20.617	3.0	ng	140528	5	21.445	949527	20.0
Heptacosane	21.105	4.2	ng	198944	5	21.445	949527	20.0
Heneicosane	21.622	6.3	ng	298268	5	21.445	949527	20.0
Bis(2-ethylhexy...	21.939	4.8	ng	227286	5	21.445	949527	20.0
Borane, diethyl...	22.197	7.6	ng	360088	5	21.445	949527	20.0
Pentadecane, 8-...	22.849	7.2	ng	343459	5	21.445	949527	20.0
Hexacosane	23.613	5.2	ng	326760	6	24.518	1265280	20.0