

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
 Data File : BG058560.D
 Acq On : 1 Aug 2023 13:17
 Operator : MA/JU
 Sample : 03769-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-P30A

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: BG058560.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.692	266	273	281	rBV6	6858	22458	1.04%	0.133%
2	5.385	384	391	405	rBV	676789	1054863	48.85%	6.230%
3	6.983	655	663	674	rBV	642193	1100457	50.96%	6.499%
4	7.812	798	804	816	rBV	204363	345839	16.02%	2.043%
5	8.975	995	1002	1015	rBV	369935	676000	31.31%	3.993%
6	10.132	1193	1199	1204	rBV5	16158	27487	1.27%	0.162%
7	10.614	1273	1281	1295	rBV	292427	524635	24.30%	3.099%
8	13.082	1693	1701	1712	rBV	973117	1523953	70.58%	9.001%
9	13.775	1814	1819	1826	rVB3	40034	60583	2.81%	0.358%
10	13.910	1836	1842	1850	rBV	146847	219727	10.18%	1.298%
11	14.416	1922	1928	1930	rBV2	36112	53299	2.47%	0.315%
12	14.463	1930	1936	1944	rVB	475784	770142	35.67%	4.549%
13	15.949	2180	2189	2199	rBV	794878	1237352	57.30%	7.308%
14	17.101	2381	2385	2393	rBV4	18305	33230	1.54%	0.196%
15	17.206	2393	2403	2414	rBV	608413	941680	43.61%	5.562%
16	17.982	2528	2535	2539	rBV5	16482	31337	1.45%	0.185%
17	18.041	2541	2545	2550	rBV	39861	58888	2.73%	0.348%
18	18.094	2550	2554	2564	rBV	274916	432210	20.02%	2.553%
19	18.399	2598	2606	2613	rBV10	15284	44505	2.06%	0.263%
20	18.816	2670	2677	2683	rVB	31608	53023	2.46%	0.313%
21	19.139	2727	2732	2737	rBV7	15965	32557	1.51%	0.192%
22	19.204	2739	2743	2746	rVV3	55872	84142	3.90%	0.497%
23	19.263	2749	2753	2766	rVV3	59204	174637	8.09%	1.031%
24	19.374	2768	2772	2781	rVB2	54743	91051	4.22%	0.538%
25	19.627	2811	2815	2821	rVB	35493	52337	2.42%	0.309%
26	19.827	2843	2849	2859	rBV	1603694	2159300	100.00%	12.753%
27	20.127	2896	2900	2909	rVB3	23528	37216	1.72%	0.220%
28	20.456	2953	2956	2960	rBV4	16286	23192	1.07%	0.137%
29	21.114	3063	3068	3089	rVB3	88556	355032	16.44%	2.097%
30	21.448	3117	3125	3131	rBV2	578884	1012657	46.90%	5.981%
31	21.854	3191	3194	3198	rVB4	25981	33387	1.55%	0.197%
32	22.201	3248	3253	3257	rBV	64062	95313	4.41%	0.563%
33	22.259	3259	3263	3264	rBV4	20080	27813	1.29%	0.164%
34	23.188	3415	3421	3430	rVB2	91294	185834	8.61%	1.098%
35	23.611	3487	3493	3503	rVB	173156	367243	17.01%	2.169%
36	23.722	3506	3512	3533	rVB	36876	213476	9.89%	1.261%

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37	24.515	3637	3647	3660	rBV2	404611	1134812	52.55%	6.702%
38	24.997	3721	3729	3741	rVB2	132594	342507	15.86%	2.023%
39	25.567	3816	3826	3840	rVB2	356911	1048967	48.58%	6.195%
40	25.755	3849	3858	3860	rBV9	29477	80110	3.71%	0.473%
41	27.588	4163	4170	4182	rVB5	44370	168243	7.79%	0.994%

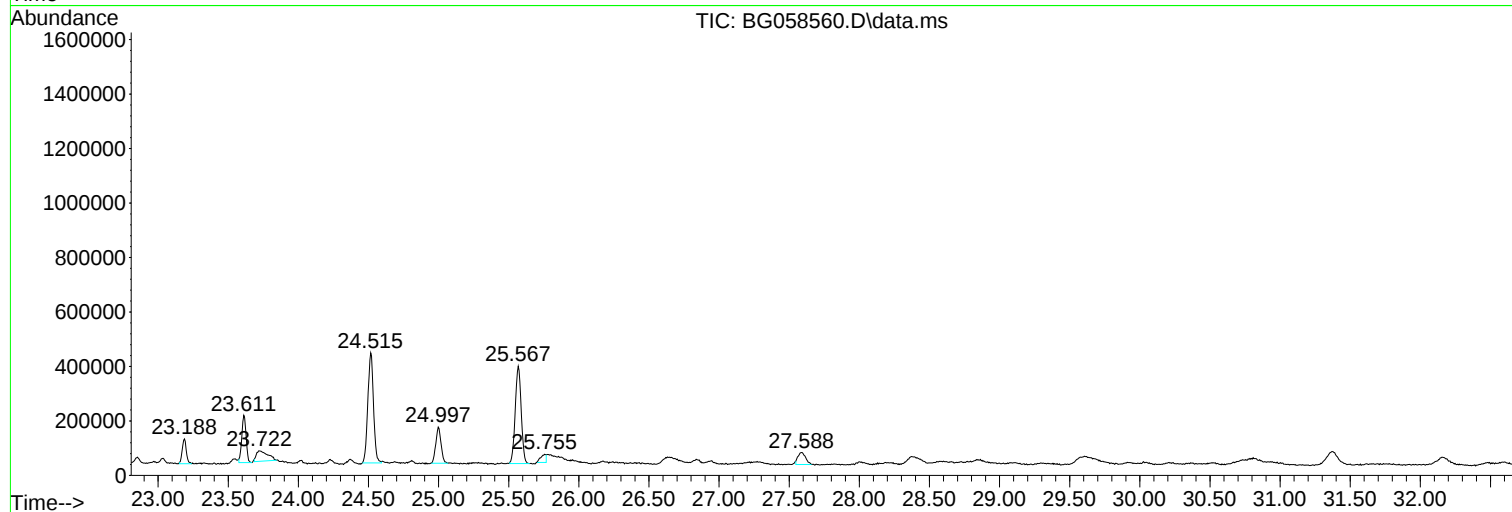
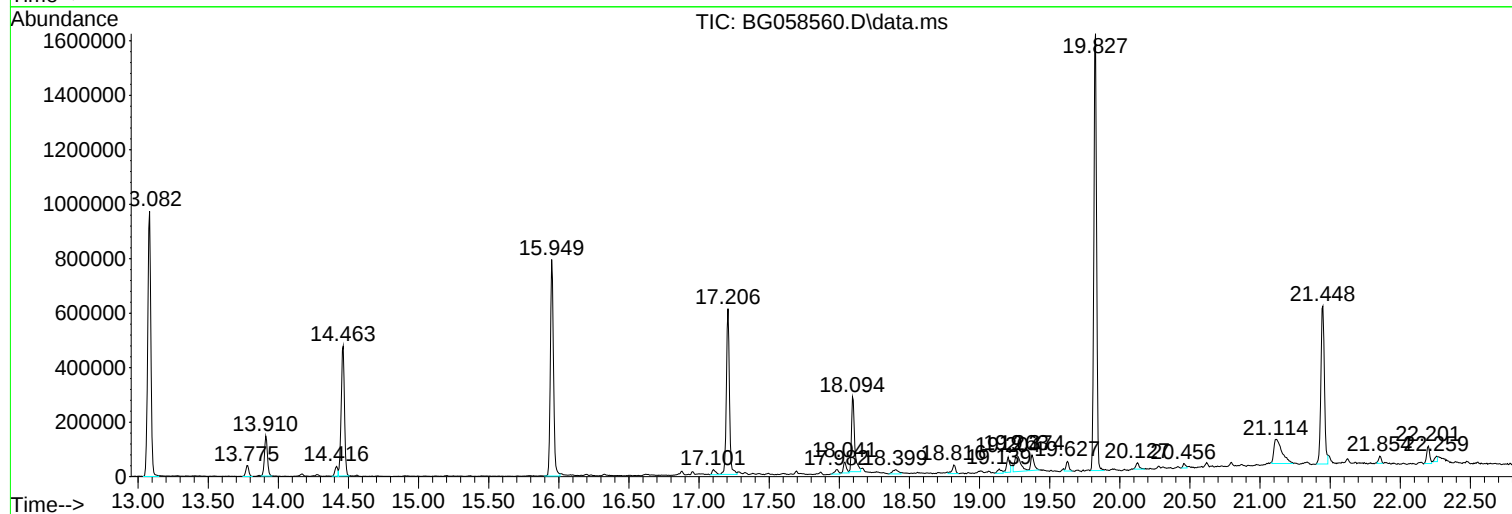
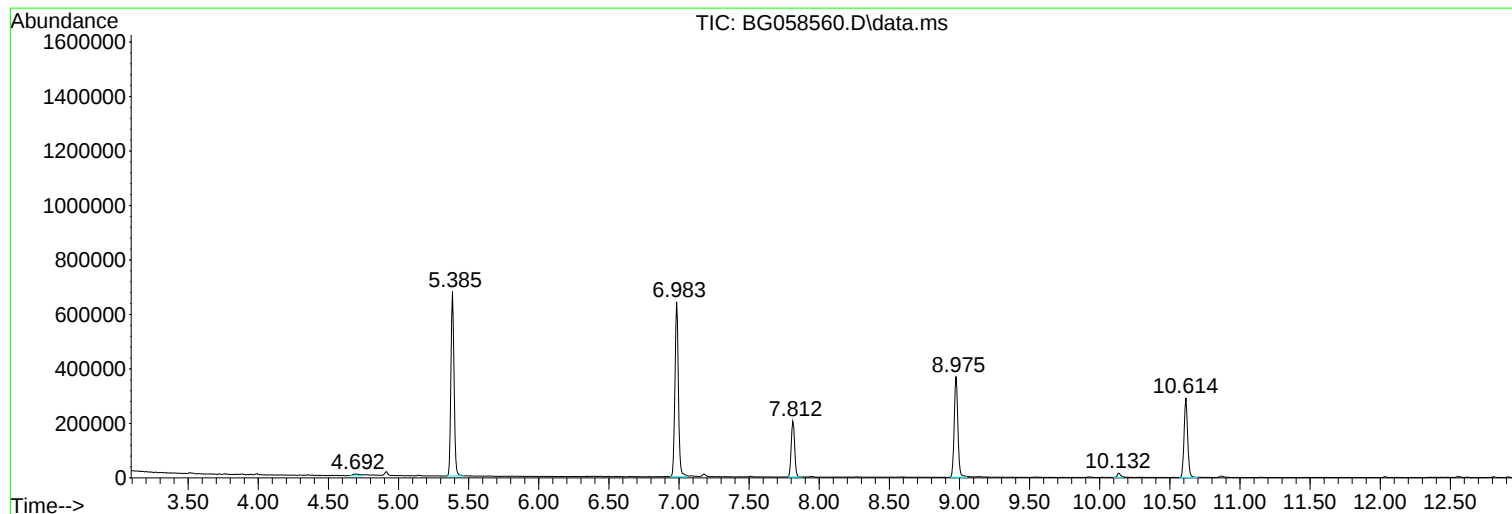
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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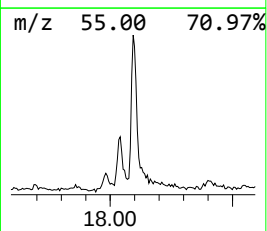
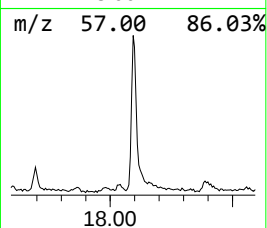
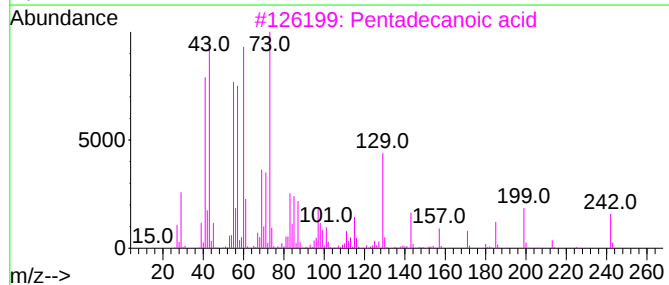
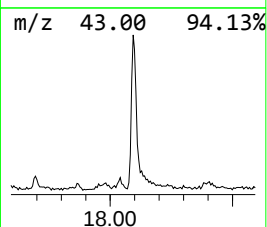
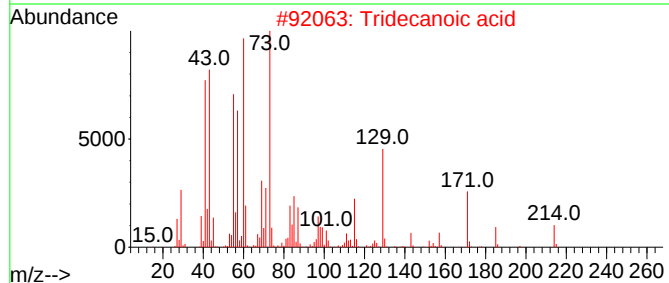
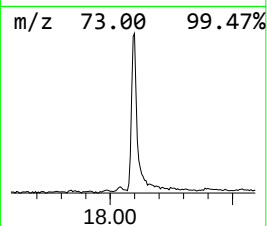
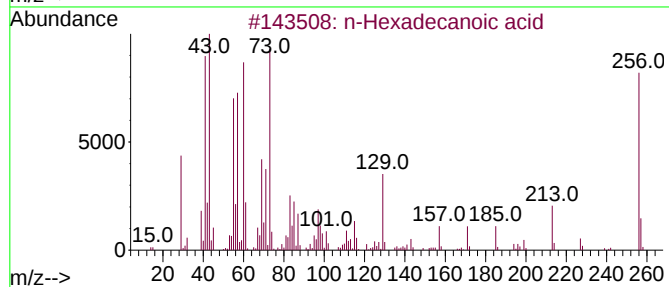
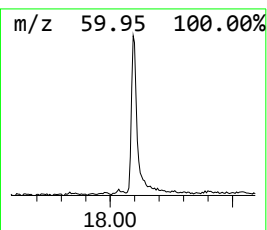
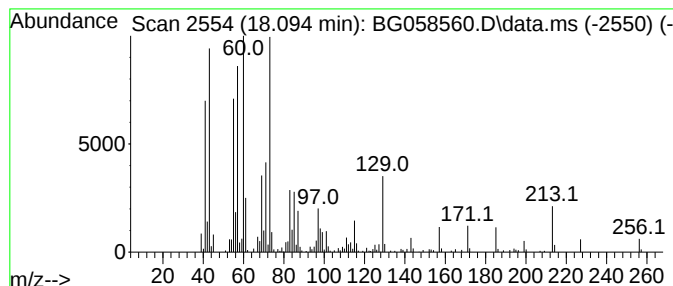
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.094	9.18 ng	432210	Phenanthrene-d10	17.206	
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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Undecanoic acid	186	C11H22O2	000112-37-8	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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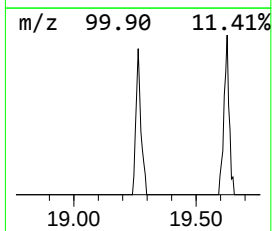
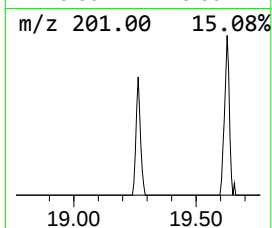
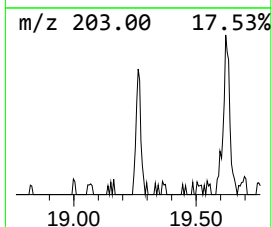
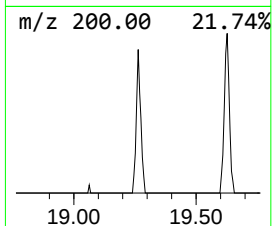
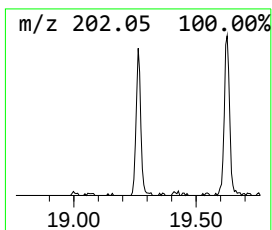
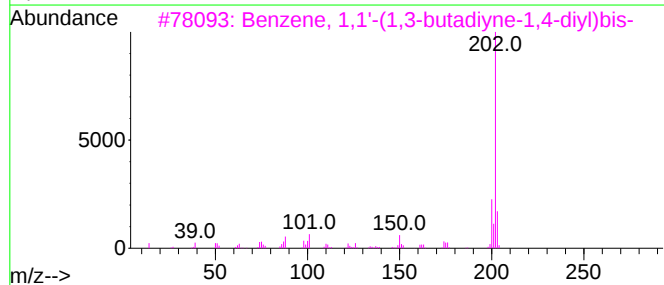
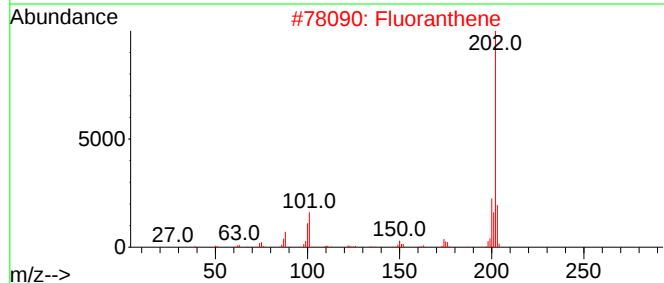
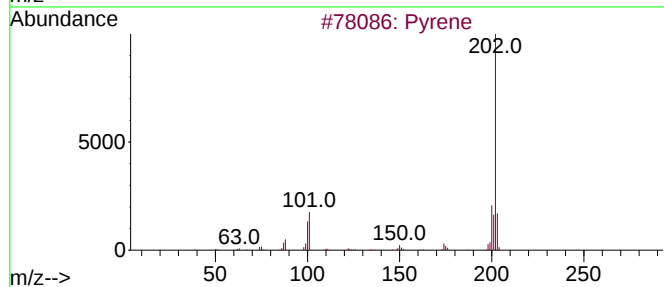
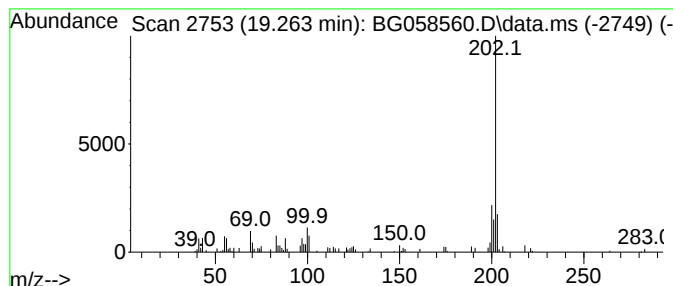
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.263	3.71 ng	174637	Phenanthrene-d10	17.206	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	81
2	Fluoranthene	202	C16H10	000206-44-0	81
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	70
4	4,5-Dihydronaphtho(2,1-d)thiazol...	202	C11H10N2S	034176-49-3	53
5	2-pyrazinol, 3-bromo-5,6-dimethyl-	202	C6H7BrN2O	1010396-05-3	38



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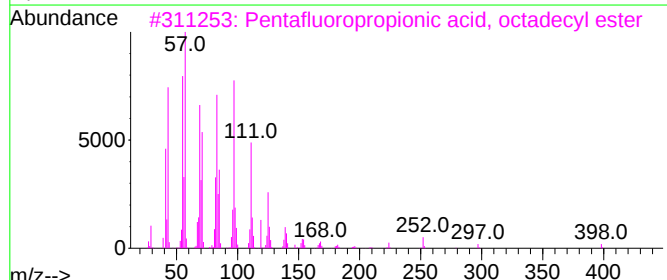
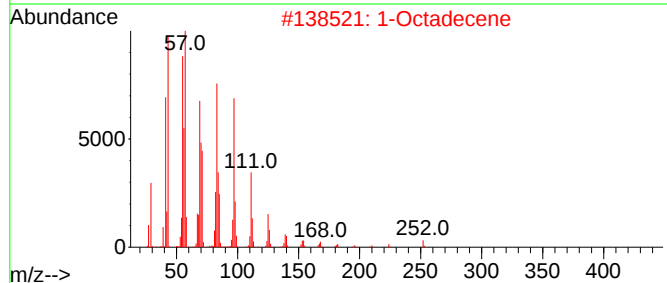
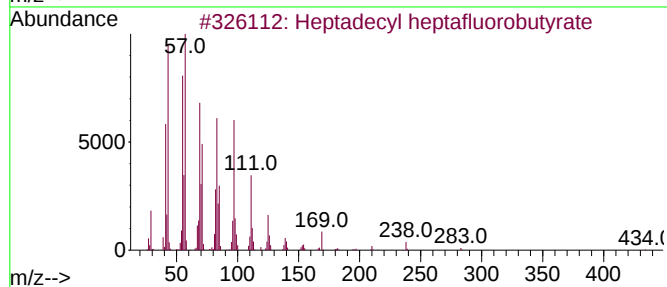
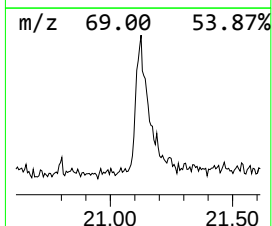
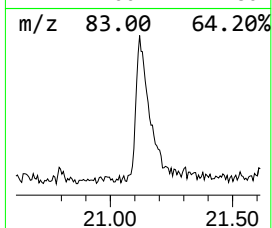
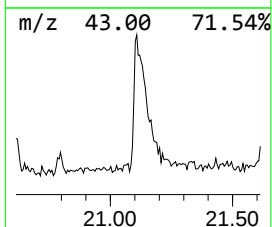
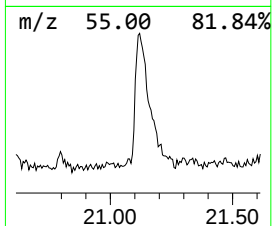
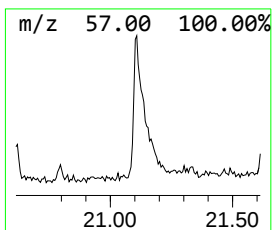
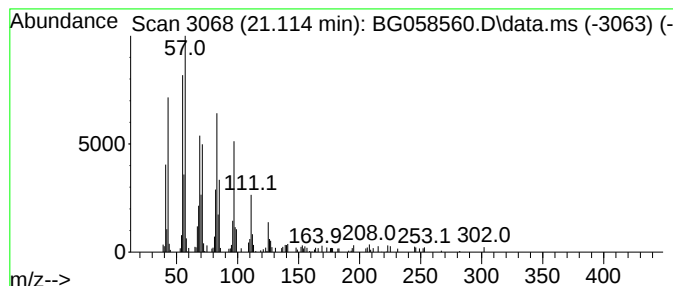
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.114	7.01 ng	355032	Chrysene-d12	21.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2			1-Octadecene	252	C18H36	000112-88-9	92
3			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91



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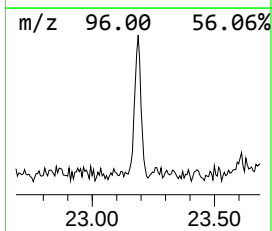
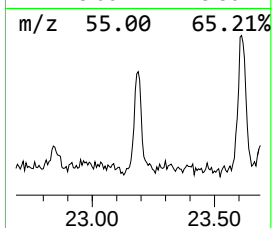
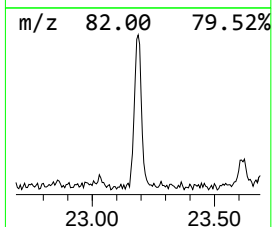
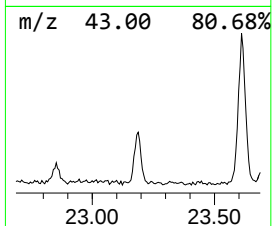
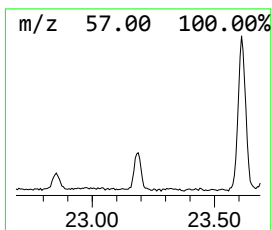
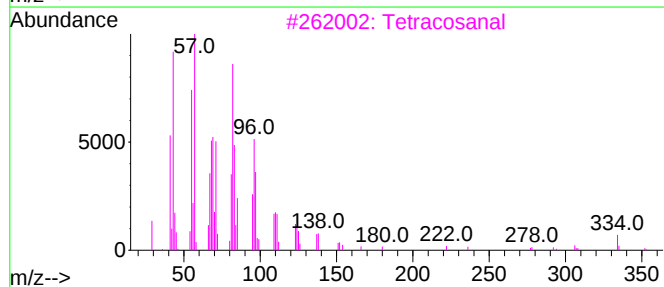
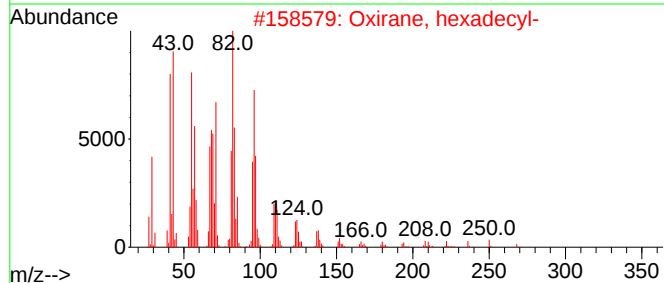
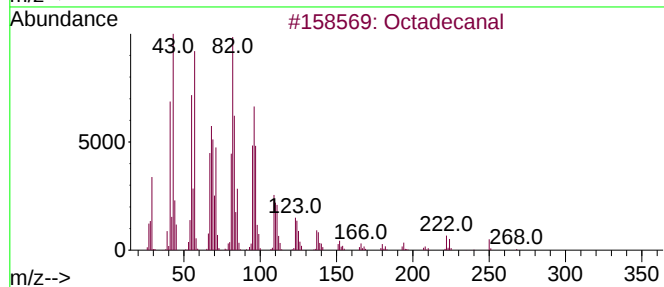
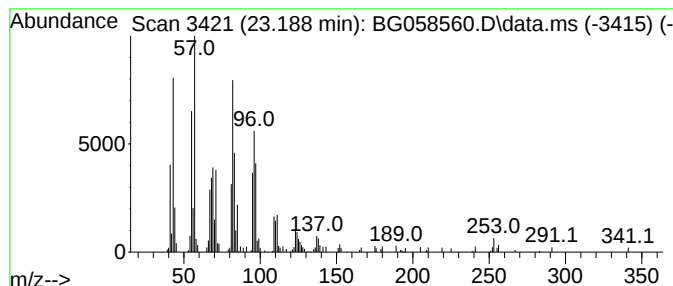
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Peak Number 4 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.188	3.28 ng	185834	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	91
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
3			Tetracosanal	352	C24H48O	057866-08-7	87
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
5			Eicosanal-	296	C20H40O	002400-66-0	74



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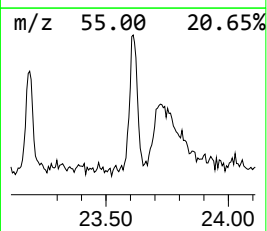
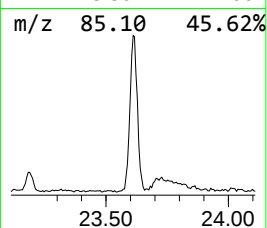
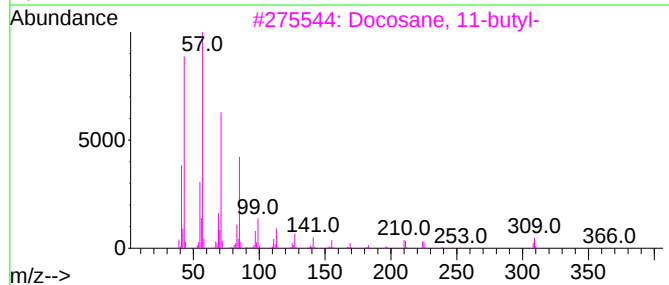
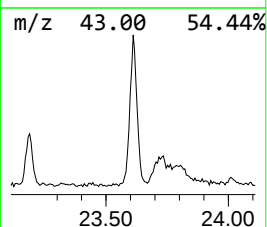
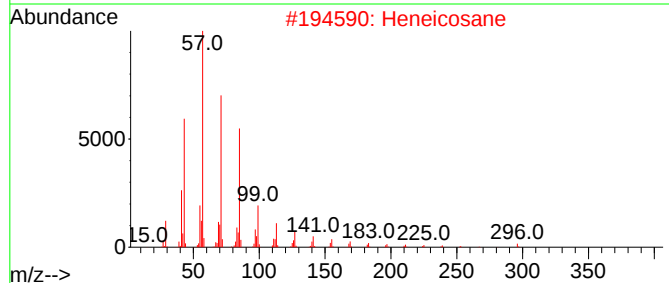
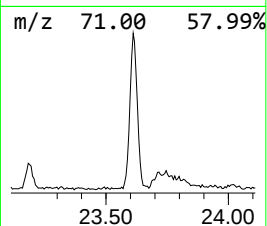
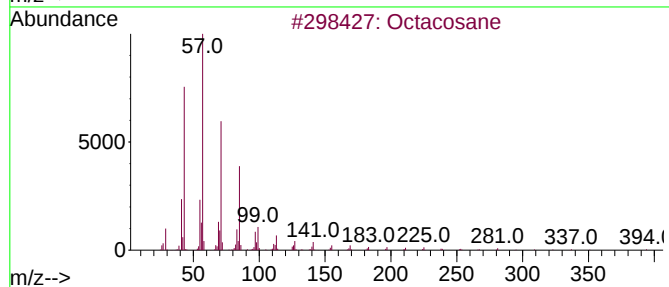
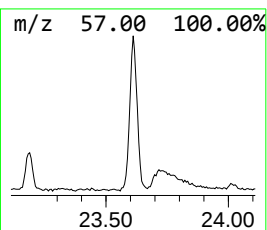
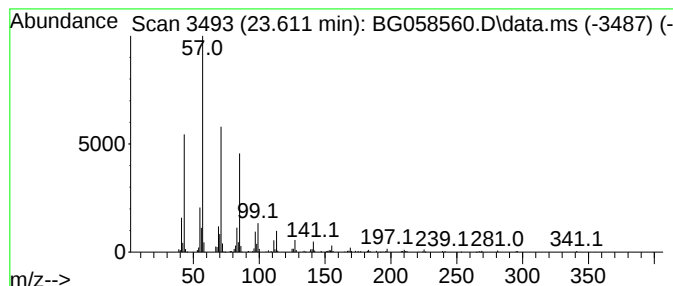
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.611	6.47 ng	367243	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058560.D
Acq On : 1 Aug 2023 13:17
Operator : MA/JU
Sample : 03769-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P30A

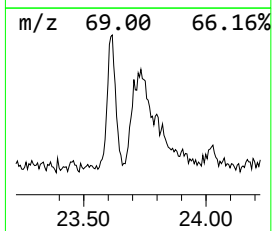
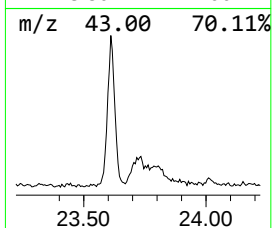
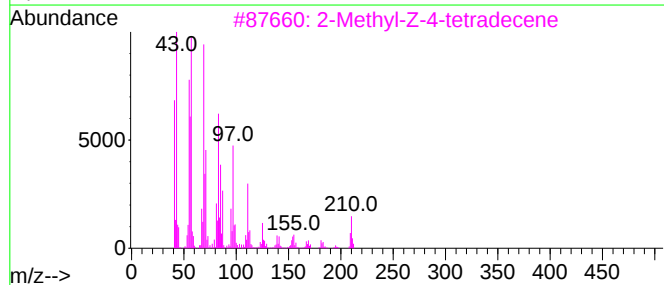
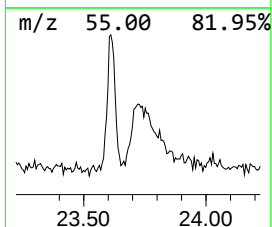
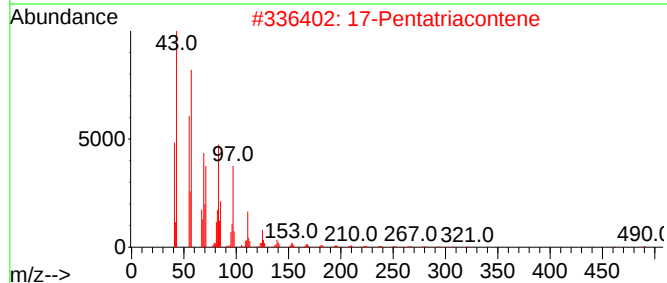
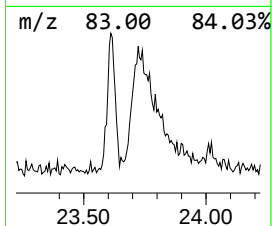
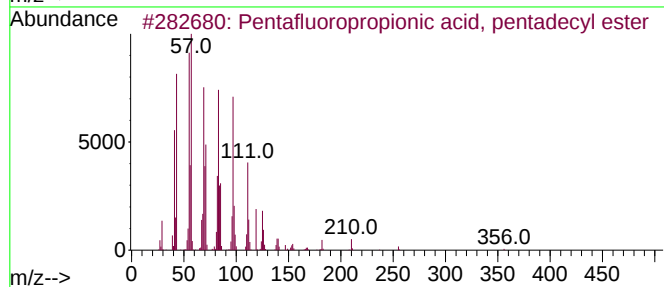
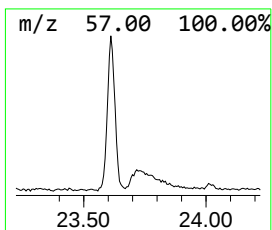
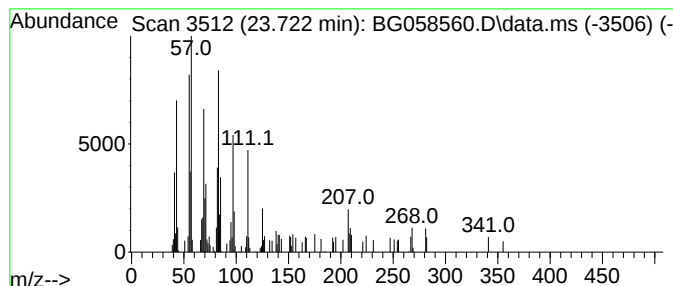
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.722	3.76 ng	213476	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	58
2			17-Pentatriacontene	491	C35H70	006971-40-0	52
3			2-Methyl-Z-4-tetradecene	210	C15H30	1000130-78-3	46
4			1-Hexacosene	364	C26H52	018835-33-1	43
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058560.D
Acq On : 1 Aug 2023 13:17
Operator : MA/JU
Sample : 03769-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

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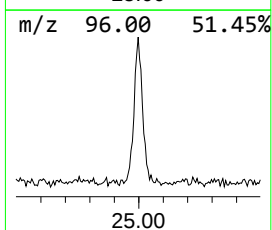
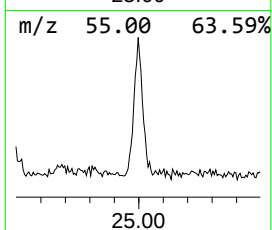
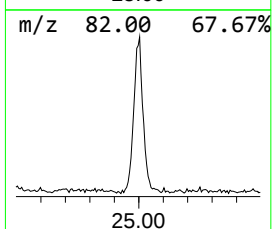
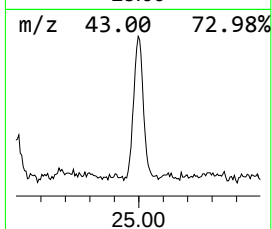
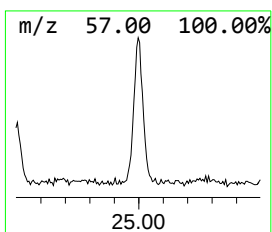
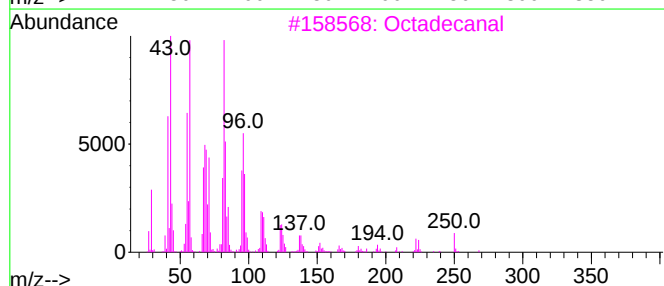
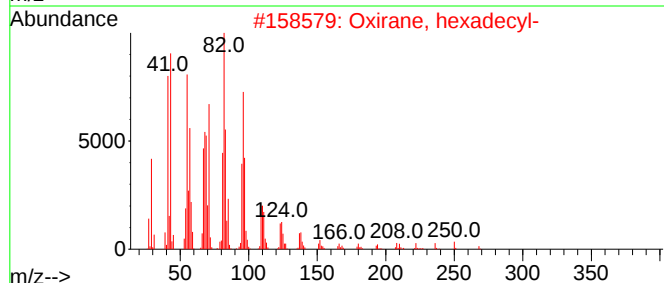
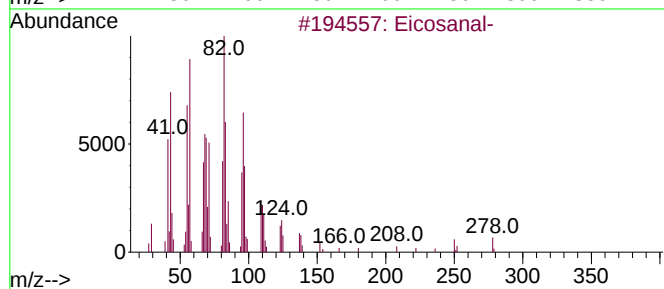
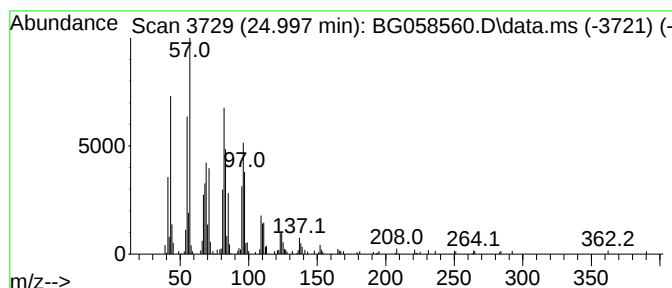
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosanal- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.997	6.04 ng	342507	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanal-	296	C20H40O	002400-66-0	91
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3			Octadecanal	268	C18H36O	000638-66-4	91
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
5			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058560.D
Acq On : 1 Aug 2023 13:17
Operator : MA/JU
Sample : 03769-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P30A

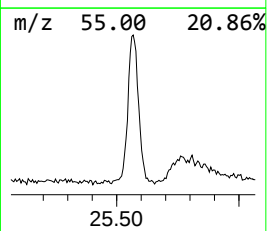
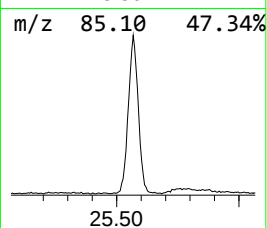
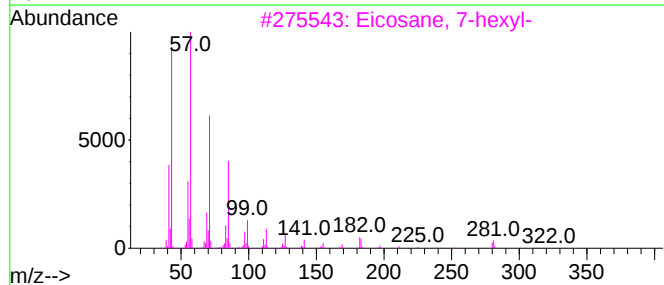
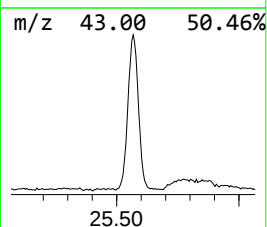
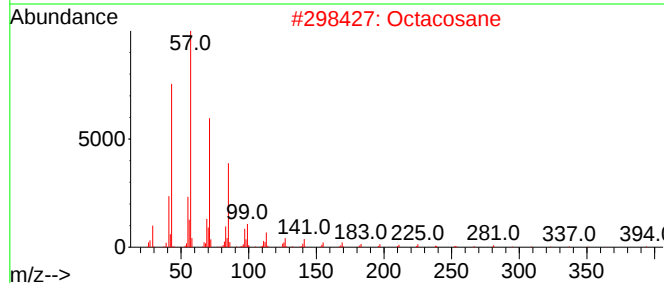
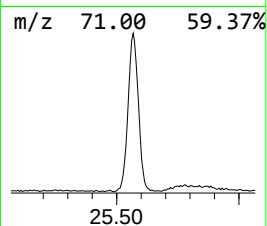
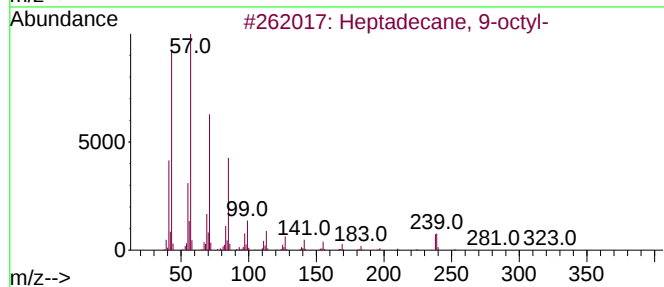
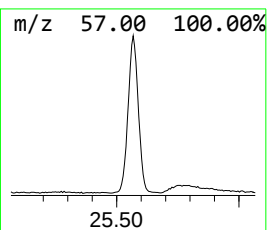
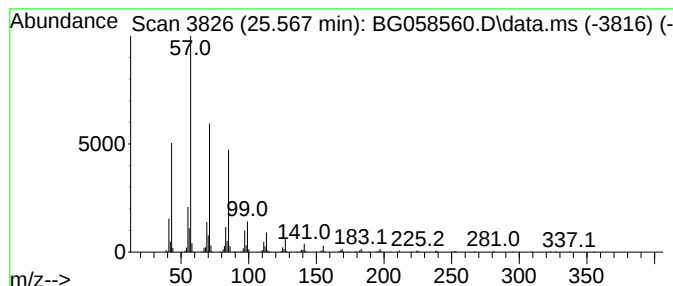
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.567	18.49 ng	1048970	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4			Heneicosane	296	C21H44	000629-94-7	90
5			Triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058560.D
Acq On : 1 Aug 2023 13:17
Operator : MA/JU
Sample : 03769-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P30A

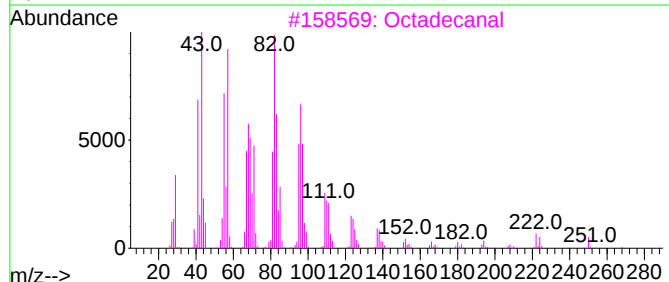
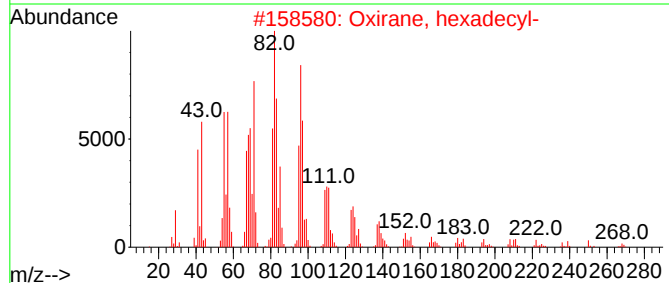
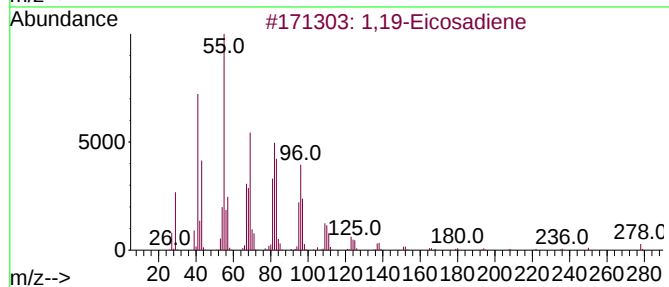
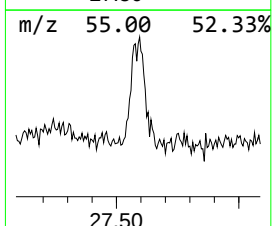
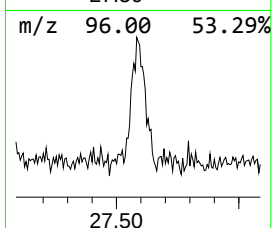
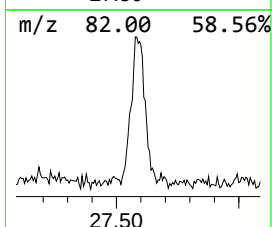
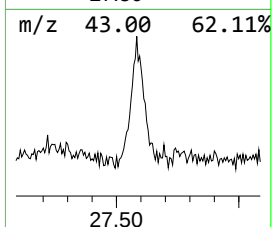
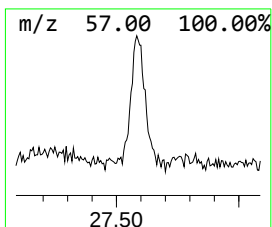
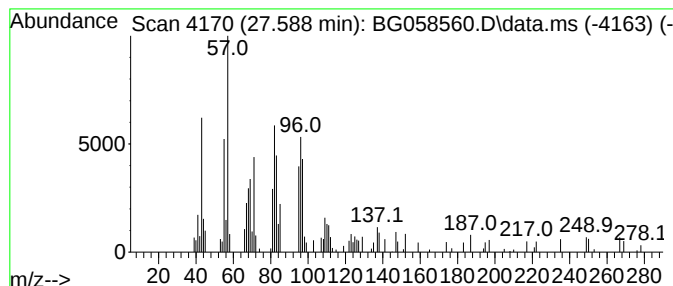
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,19-Eicosadiene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.588	2.97 ng	168243	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,19-Eicosadiene	278	C20H38	014811-95-1	78
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
3			Octadecanal	268	C18H36O	000638-66-4	72
4			1,15-Hexadecadiene	222	C16H30	021964-51-2	53
5			1,13-Tetradecadiene	194	C14H26	021964-49-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058560.D
Acq On : 1 Aug 2023 13:17
Operator : MA/JU
Sample : 03769-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P30A

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
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Benzene, 1,1'-(...	19.263	3.7	ng	174637	4	17.206	941680	20.0
Heptadecyl hept...	21.114	7.0	ng	355032	5	21.448	1012660	20.0
Octadecanal	23.188	3.3	ng	185834	6	24.515	1134810	20.0
Octacosane	23.611	6.5	ng	367243	6	24.515	1134810	20.0
Pentafluoroprop...	23.722	3.8	ng	213476	6	24.515	1134810	20.0
Eicosanal-	24.997	6.0	ng	342507	6	24.515	1134810	20.0
Heptadecane, 9-...	25.567	18.5	ng	1048970	6	24.515	1134810	20.0
1,19-Eicosadiene	27.588	3.0	ng	168243	6	24.515	1134810	20.0