

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
 Data File : BG061089.D
 Acq On : 2 May 2024 11:58
 Operator : MA/JU
 Sample : P2330-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E-2(0.5-1.5)

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-BG043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061089.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.148	23	27	33	rVB	19050	31390	2.09%	0.394%
2	3.671	112	116	127	rVB	9983	18065	1.21%	0.227%
3	5.522	424	431	440	rBV	289743	461096	30.76%	5.794%
4	7.103	692	700	710	rBV	313105	542858	36.21%	6.821%
5	7.931	835	841	848	rBV2	87182	139311	9.29%	1.750%
6	9.089	1029	1038	1047	rBV	203097	359616	23.99%	4.519%
7	10.728	1306	1317	1323	rBV	109342	195416	13.04%	2.455%
8	13.184	1728	1735	1742	rBV	562914	872310	58.19%	10.960%
9	14.559	1962	1969	1976	rBV	194004	297516	19.85%	3.738%
10	14.776	2000	2006	2011	rBV6	9025	17336	1.16%	0.218%
11	16.051	2217	2223	2235	rBV	563788	861643	57.48%	10.826%
12	17.308	2430	2437	2441	rBV	257312	381399	25.44%	4.792%
13	17.349	2441	2444	2449	rVB	36248	49196	3.28%	0.618%
14	18.207	2581	2590	2600	rBV3	63489	132014	8.81%	1.659%
15	18.378	2614	2619	2623	rBV4	21543	38997	2.60%	0.490%
16	18.413	2623	2625	2632	rVB5	12518	17783	1.19%	0.223%
17	19.095	2737	2741	2746	rBV6	11679	19777	1.32%	0.248%
18	19.359	2781	2786	2792	rBV	124310	182306	12.16%	2.291%
19	19.424	2792	2797	2801	rBV	35941	50282	3.35%	0.632%
20	19.723	2840	2848	2857	rVB	113237	188725	12.59%	2.371%
21	19.929	2874	2883	2888	rBV	1194918	1499155	100.00%	18.837%
22	20.052	2898	2904	2906	rBV7	14838	26370	1.76%	0.331%
23	20.217	2929	2932	2935	rVB	21034	23800	1.59%	0.299%
24	20.317	2946	2949	2953	rVB2	15609	20378	1.36%	0.256%
25	20.375	2956	2959	2963	rVB2	13319	18973	1.27%	0.238%
26	20.516	2980	2983	2986	rBV	13021	15316	1.02%	0.192%
27	20.563	2988	2991	2994	rVV4	12131	17892	1.19%	0.225%
28	21.239	3102	3106	3112	rBV3	50511	96185	6.42%	1.209%
29	21.562	3154	3161	3166	rBV3	290224	551446	36.78%	6.929%
30	23.830	3541	3547	3553	rVB2	99845	203417	13.57%	2.556%
31	24.688	3685	3693	3703	rBV2	127527	380088	25.35%	4.776%
32	25.851	3883	3891	3899	rBV3	84954	248687	16.59%	3.125%

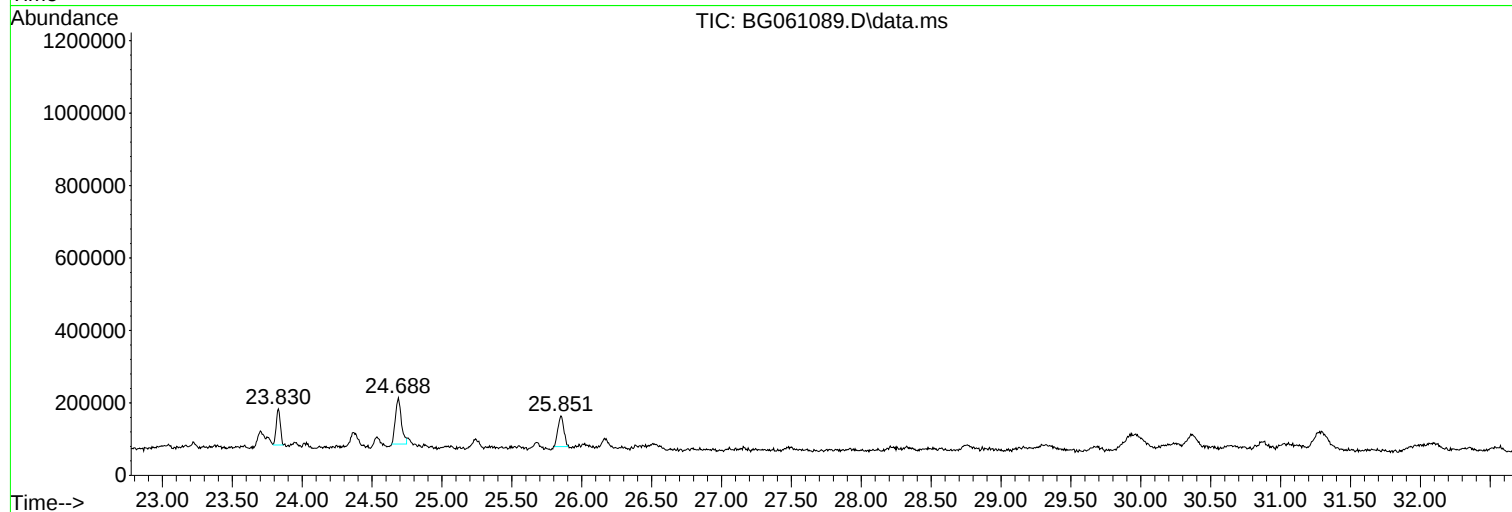
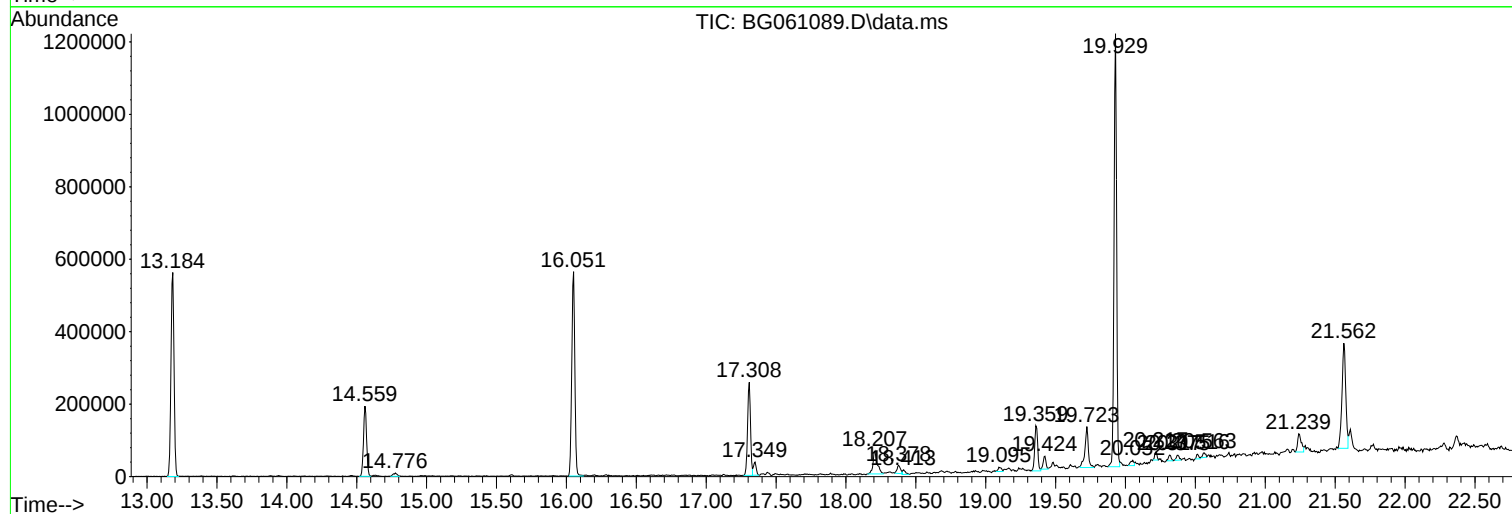
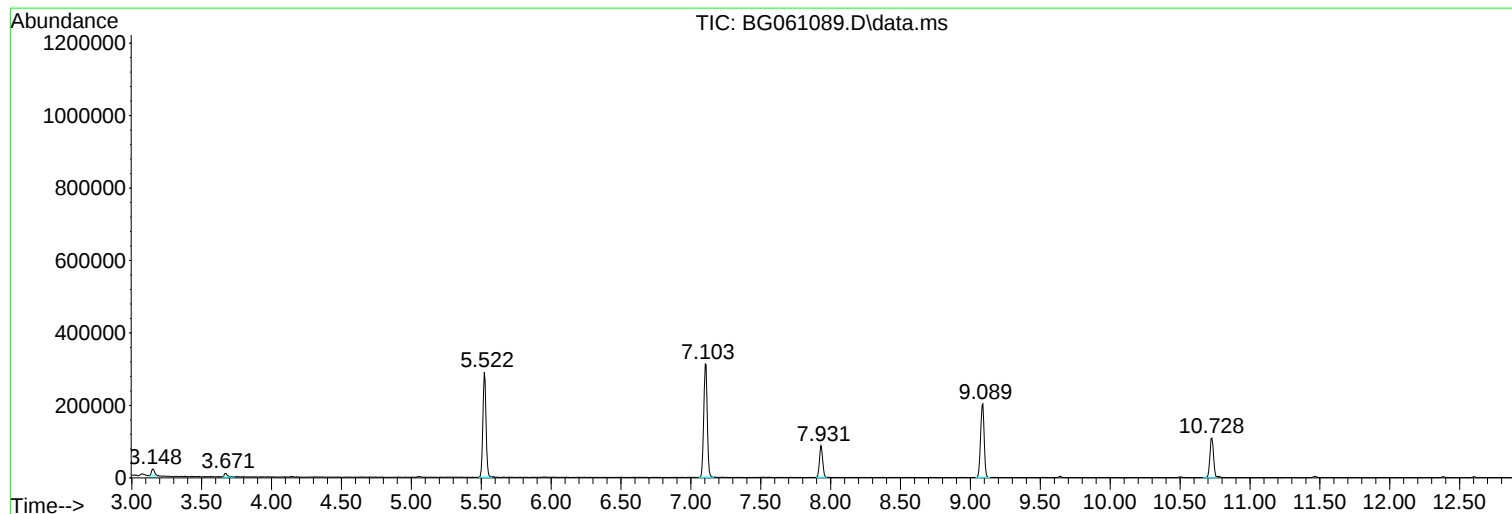
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ClientSampleId :
E-2(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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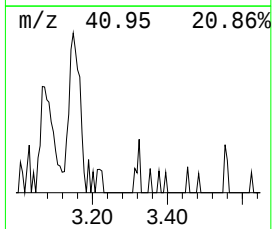
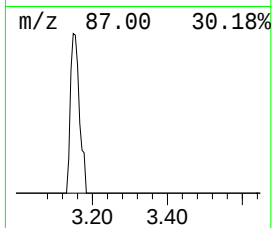
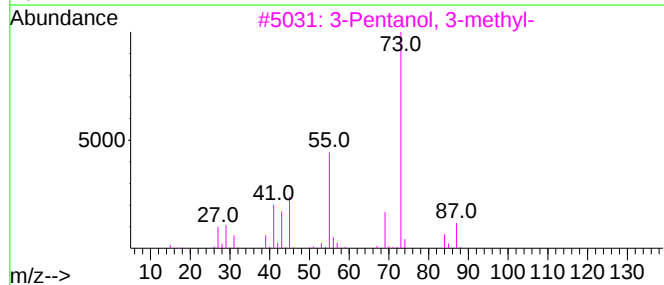
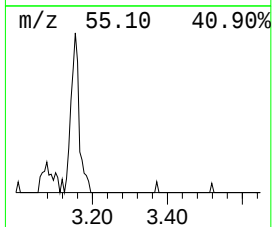
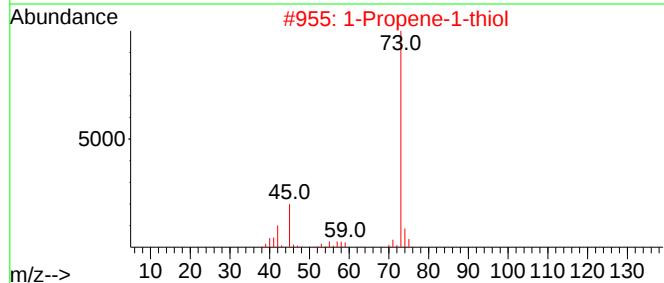
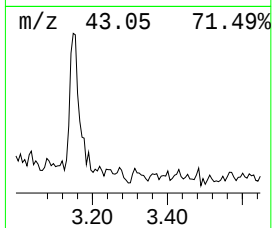
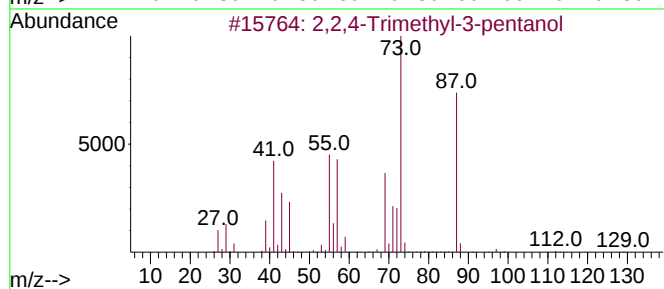
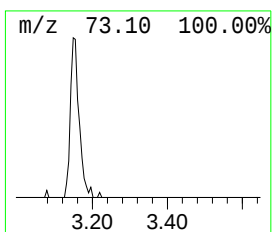
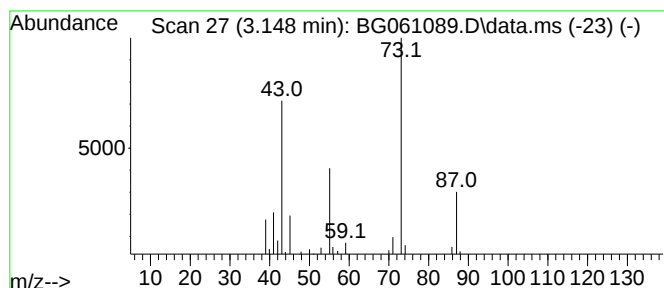
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.148 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.148	4.51 ng	31390	1,4-Dichlorobenzene-d4	7.931

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38	
2	1-Propene-1-thiol	74	C3H6S	000925-89-3	38	
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33	
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25	
5	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	17	



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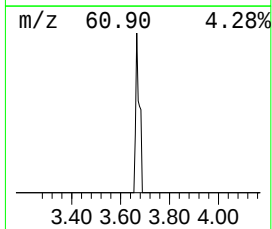
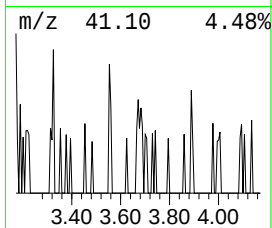
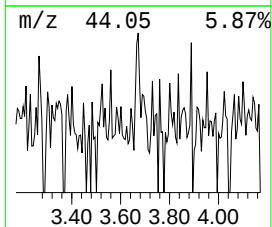
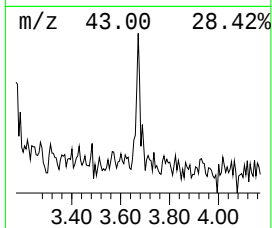
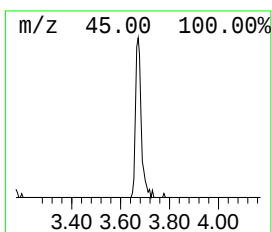
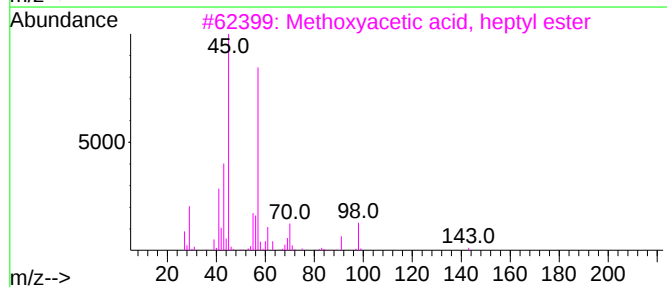
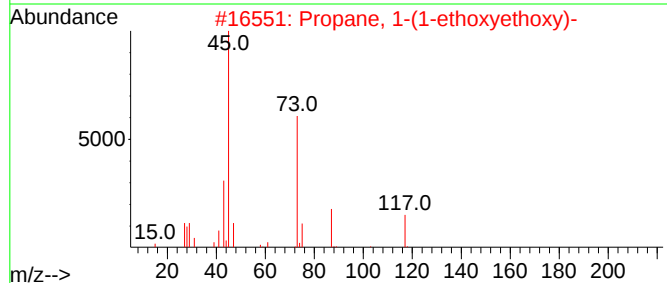
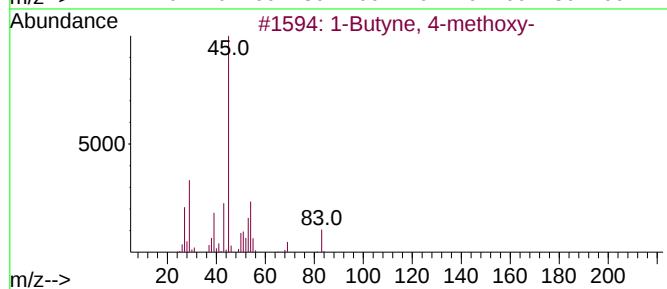
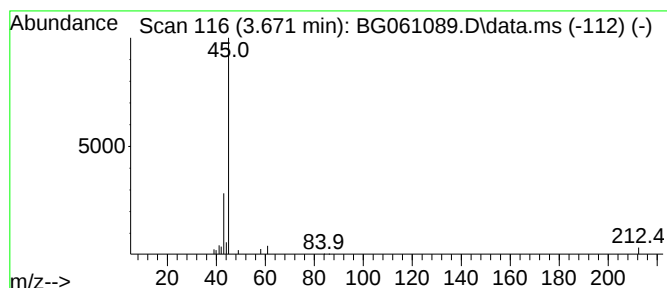
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.671 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
3.671	2.59 ng	18065	1,4-Dichlorobenzene-d4			7.931

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butyne, 4-methoxy-	84	C5H8O	036678-08-7	5
2		Propane, 1-(1-ethoxyethoxy)-	132	C7H16O2	020680-10-8	4
3		Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	4
4		Formamide	45	CH3NO	000075-12-7	3
5		2-Propanol, 1-hydrazino-	90	C3H10N2O	018501-20-7	2



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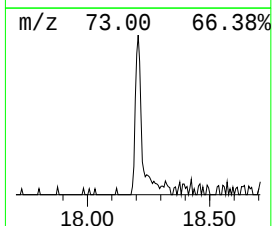
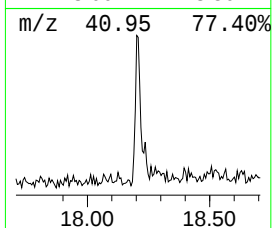
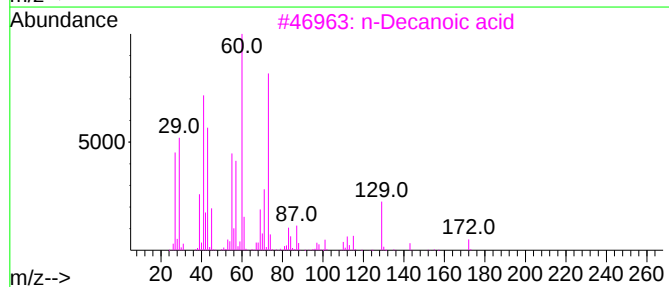
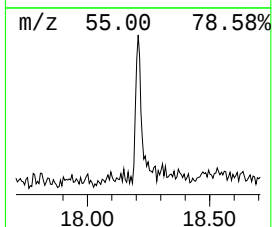
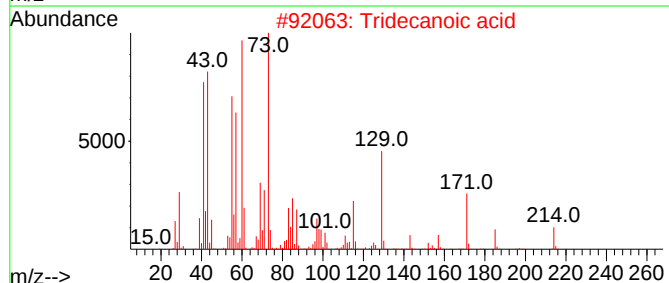
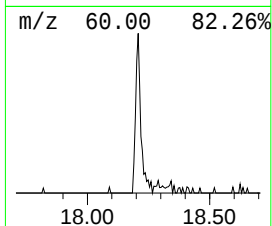
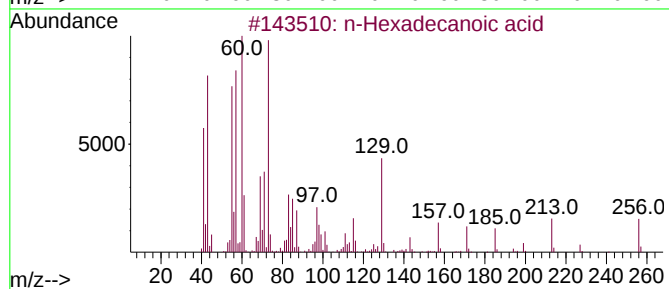
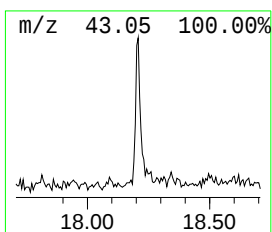
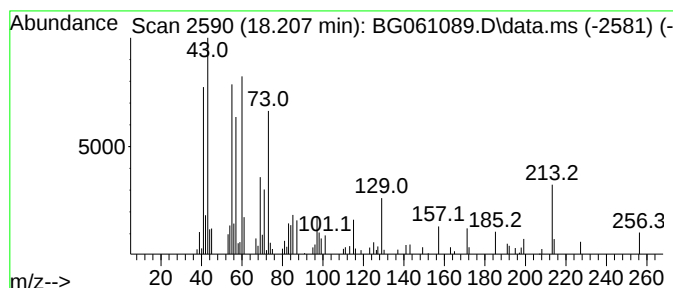
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.207	6.92 ng	132014	Phenanthrene-d10	17.308

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	70
3			n-Decanoic acid	172	C10H20O2	000334-48-5	53
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5			Undecanoic acid	186	C11H22O2	000112-37-8	46



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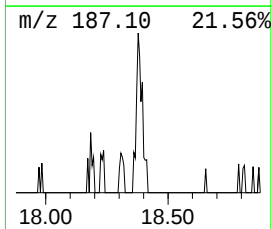
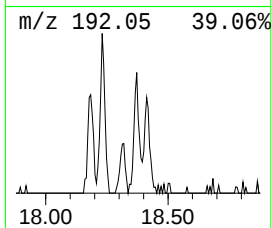
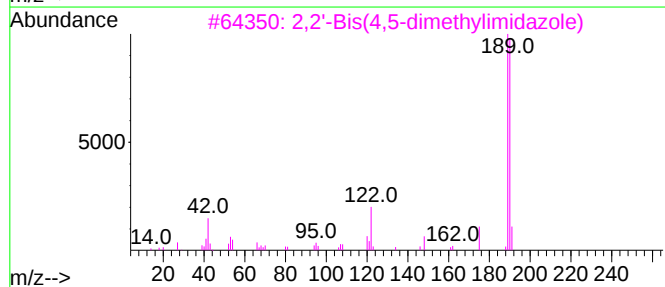
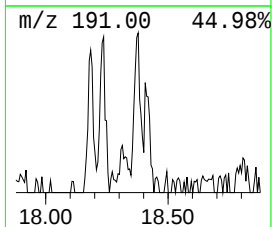
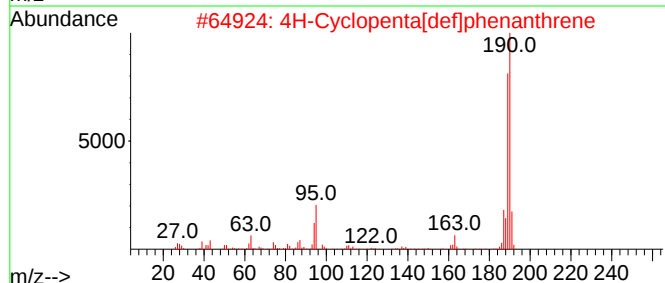
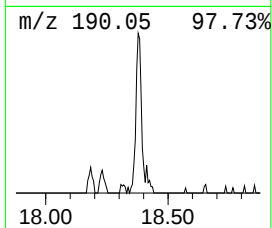
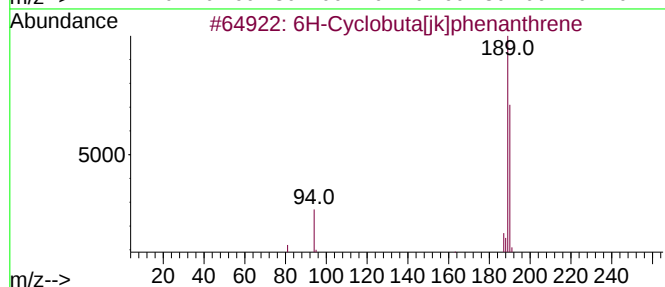
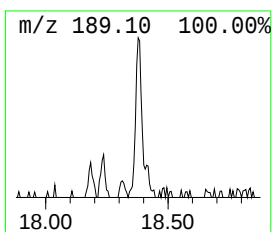
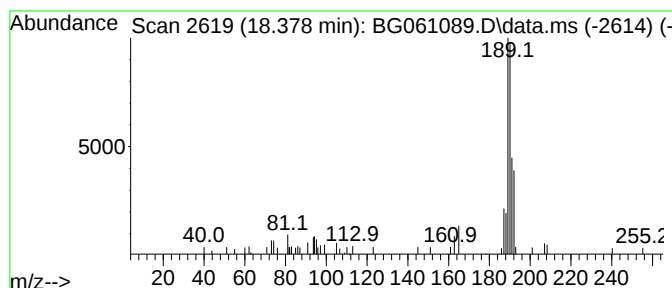
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 6H-Cyclobuta[jk]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.378	2.04 ng	38997	Phenanthrene-d10		17.308	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[jk]phenanthrene		190	C15H10	083469-43-6	58
2	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	47
3	2,2'-Bis(4,5-dimethylimidazole)		190	C10H14N4	069286-06-2	37
4	Cyclohexanone, 2-(2-furanylmethy...		190	C12H14O2	056053-07-7	27
5	4-Isothiazolecarbonitrile, 5-chl...		190	C5H3ClN2S2	054798-93-5	16



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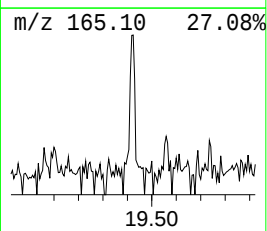
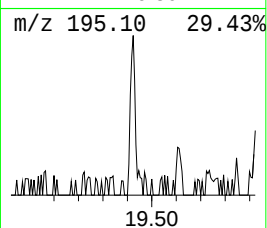
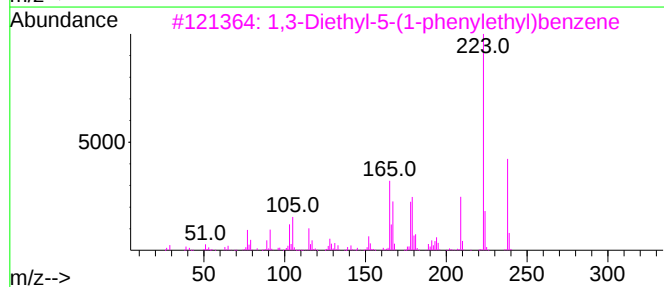
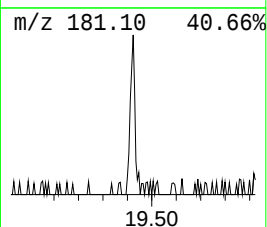
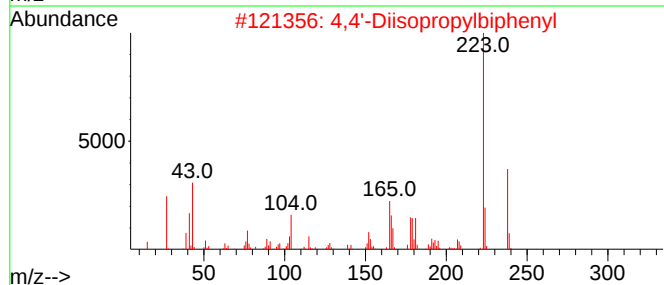
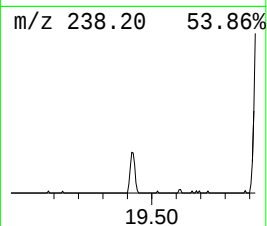
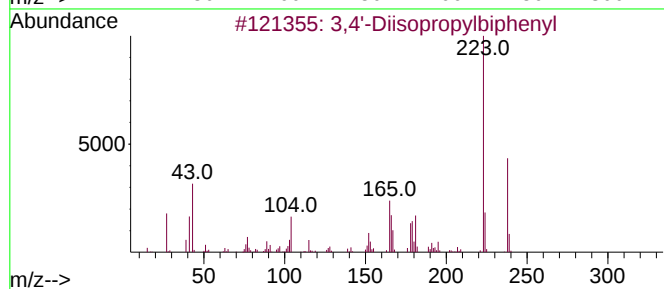
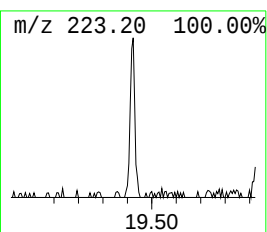
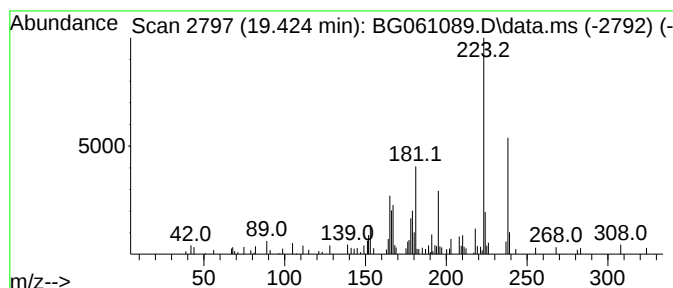
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 3,4'-Diisopropylbiphenyl Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.424	2.64 ng	50282	Phenanthrene-d10	17.308

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	89
2			4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	89
3			1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	76
4			10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	53
5			4-tert-Butylbenzenethiol, S-trim...	238	C13H22SSi	123045-43-2	49



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
E-2(0.5-1.5)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

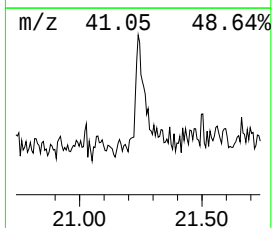
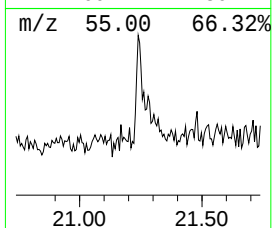
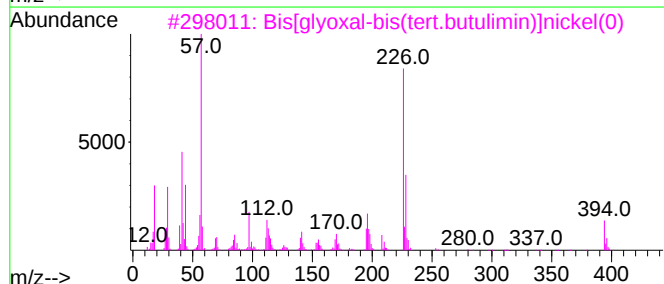
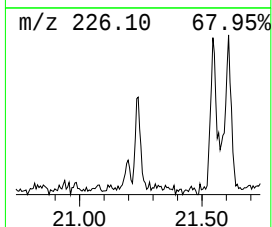
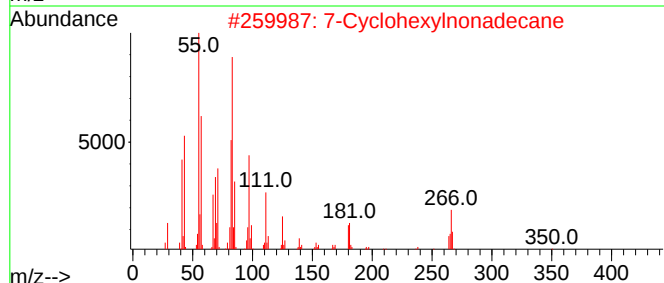
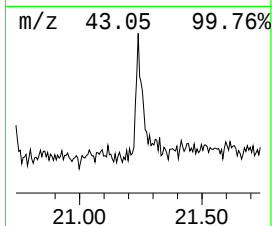
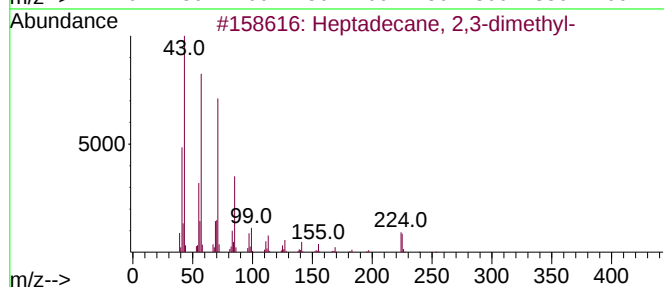
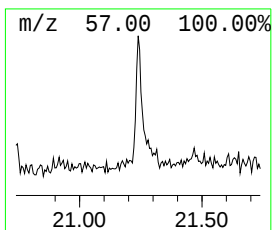
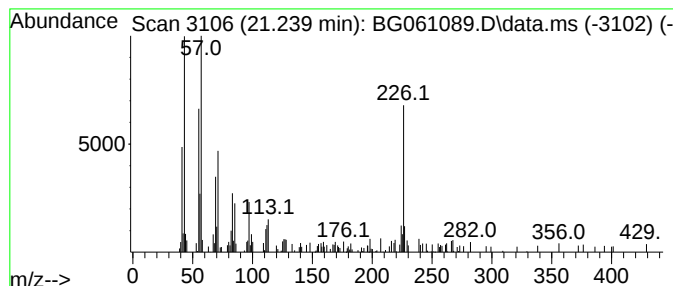
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown21.239 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.239	3.49 ng	96185	Chrysene-d12	21.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,3-dimethyl-	268	C19H40	061868-03-9	35
2		7-Cyclohexylnonadecane	350	C25H50	1010357-25-4	27
3		Bis[glyoxal-bis(tert.butulimin)]...	394	C20H40N4Ni	1000286-92-6	27
4		Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	22
5		N-(2-Methyl-5-oxo-5H-chromeno[3,...	282	C16H14N2O3	1000295-08-0	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061089.D
Acq On : 2 May 2024 11:58
Operator : MA/JU
Sample : P2330-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E-2(0.5-1.5)

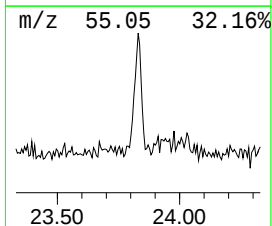
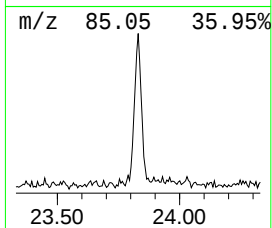
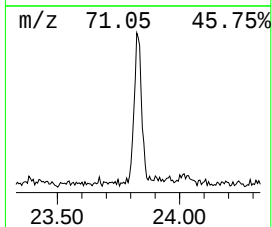
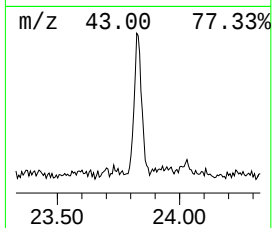
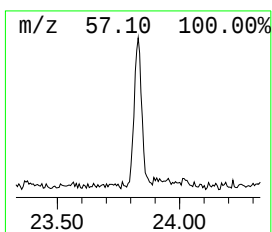
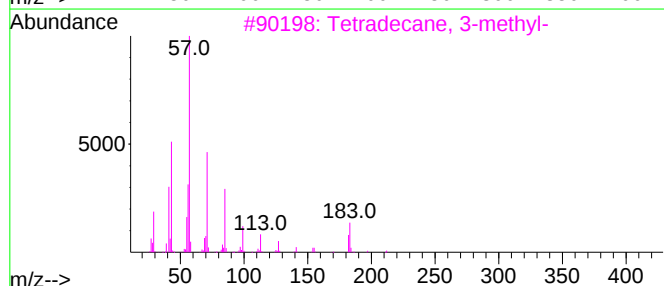
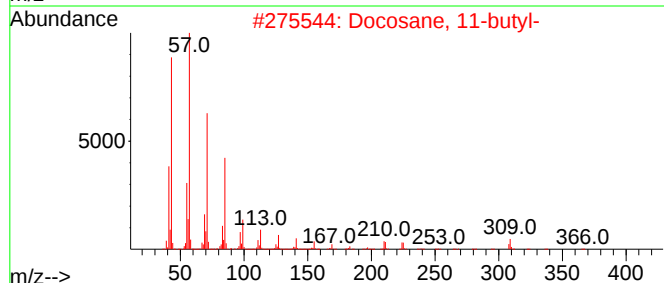
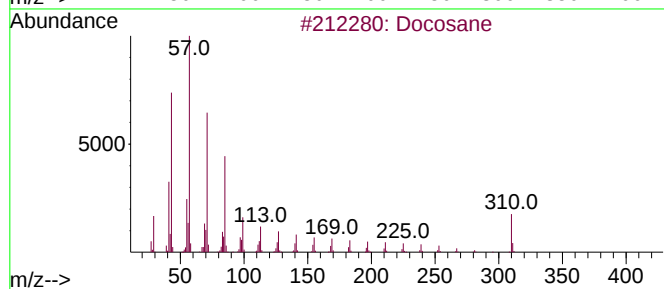
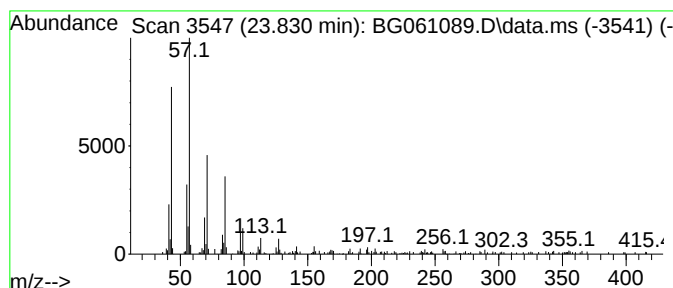
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.830	10.70 ng	203417	Perylene-d12	24.688

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	90
2			Docosane, 11-butyl-	366	C26H54	013475-76-8	83
3			Tetradecane, 3-methyl-	212	C15H32	018435-22-8	81
4			Dotriacontane	451	C32H66	000544-85-4	80
5			Hentriacontane	437	C31H64	000630-04-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061089.D
Acq On : 2 May 2024 11:58
Operator : MA/JU
Sample : P2330-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E-2(0.5-1.5)

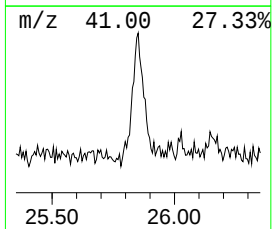
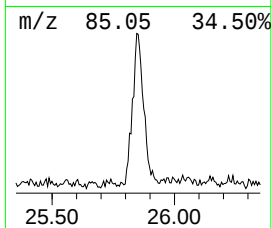
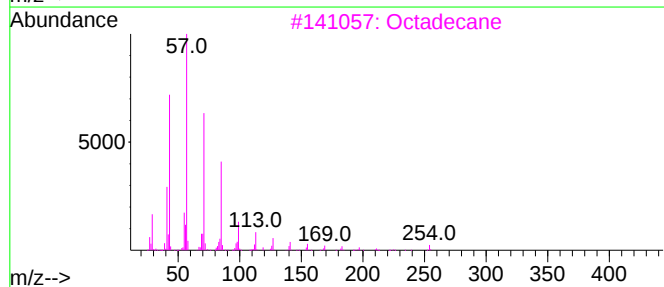
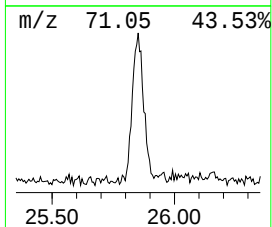
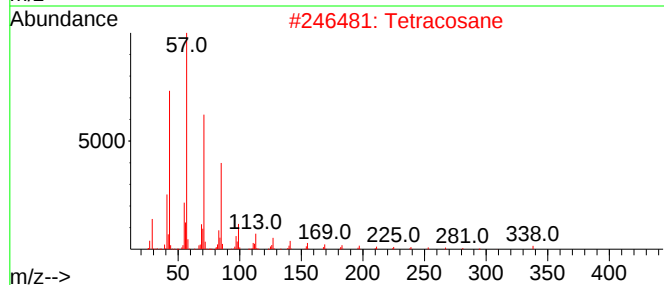
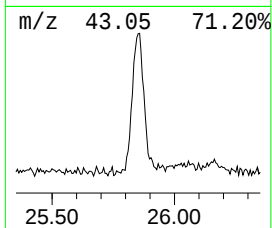
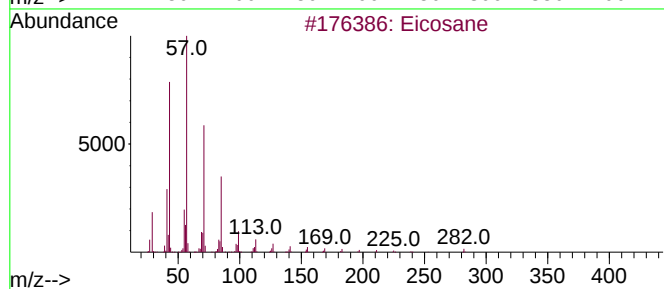
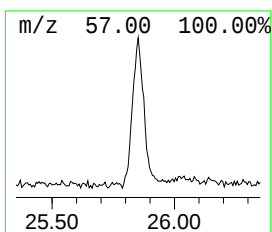
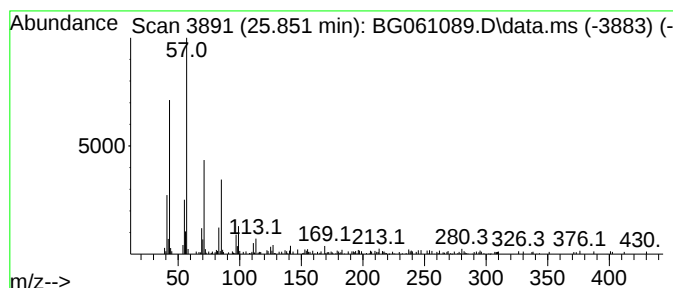
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.851	13.09 ng	248687	Perylene-d12	24.688

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	93
2	Tetracosane			338	C24H50	000646-31-1	93
3	Octadecane			254	C18H38	000593-45-3	93
4	Heneicosane			296	C21H44	000629-94-7	93
5	Pentadecane			212	C15H32	000629-62-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061089.D
Acq On : 2 May 2024 11:58
Operator : MA/JU
Sample : P2330-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E-2(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.148	3.148	4.5	ng	31390	1	7.931	139311	20.0
unknown3.671	3.671	2.6	ng	18065	1	7.931	139311	20.0
n-Hexadecanoic ...	18.207	6.9	ng	132014	4	17.308	381399	20.0
6H-Cyclobuta[jk...	18.378	2.0	ng	38997	4	17.308	381399	20.0
3,4'-Diisopropy...	19.424	2.6	ng	50282	4	17.308	381399	20.0
unknown21.239	21.239	3.5	ng	96185	5	21.562	551446	20.0
Docosane	23.830	10.7	ng	203417	6	24.688	380088	20.0
Eicosane	25.851	13.1	ng	248687	6	24.688	380088	20.0