

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
 Data File : BF124062.D
 Acq On : 26 May 2021 13:32
 Operator : JU/CG
 Sample : M2516-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1-5-TP

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_F\METHODS\8270-BF051421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	11	19	24	rBV	609320	745492	33.63%	5.248%
2	2.305	31	37	43	rBV	37184	48055	2.17%	0.338%
3	5.116	510	515	525	rVB	454646	597737	26.96%	4.208%
4	5.522	578	584	587	rBV	1469173	1398427	63.08%	9.845%
5	5.910	646	650	655	rVB	51577	46527	2.10%	0.328%
6	6.522	748	754	757	rBV	1432338	1424572	64.25%	10.029%
7	6.722	786	788	798	rBV3	12561	26254	1.18%	0.185%
8	6.892	813	817	820	rBV	424783	328318	14.81%	2.311%
9	7.451	907	912	916	rBV	954634	996718	44.96%	7.017%
10	8.175	1031	1035	1039	rBV	508059	427211	19.27%	3.008%
11	9.251	1213	1218	1221	rBV	2269070	1860562	83.92%	13.098%
12	9.363	1234	1237	1241	rVB	21871	22863	1.03%	0.161%
13	9.639	1281	1284	1289	rVB	156974	129920	5.86%	0.915%
14	9.933	1330	1334	1337	rBV	585892	506968	22.87%	3.569%
15	10.722	1464	1468	1471	rBV	1559787	1357825	61.24%	9.559%
16	11.422	1582	1587	1590	rBV	683430	554500	25.01%	3.904%
17	11.945	1671	1676	1680	rBV	74538	84249	3.80%	0.593%
18	13.010	1851	1857	1860	rBV	2341179	2217061	100.00%	15.608%
19	13.939	2011	2015	2029	rVB5	126304	327849	14.79%	2.308%
20	14.063	2033	2036	2040	rVB	397137	370523	16.71%	2.608%
21	14.316	2073	2079	2088	rVB3	52840	117534	5.30%	0.827%
22	14.598	2123	2127	2130	rBV6	18959	33730	1.52%	0.237%
23	15.104	2208	2213	2217	rBV4	39336	69613	3.14%	0.490%
24	15.198	2225	2229	2234	rVB5	26371	37041	1.67%	0.261%
25	15.510	2278	2282	2285	rBV6	22316	37291	1.68%	0.263%
26	15.563	2285	2291	2298	rVB	259999	375105	16.92%	2.641%
27	16.162	2388	2393	2395	rBV5	19938	34398	1.55%	0.242%
28	17.174	2559	2565	2572	rVB10	11793	28251	1.27%	0.199%

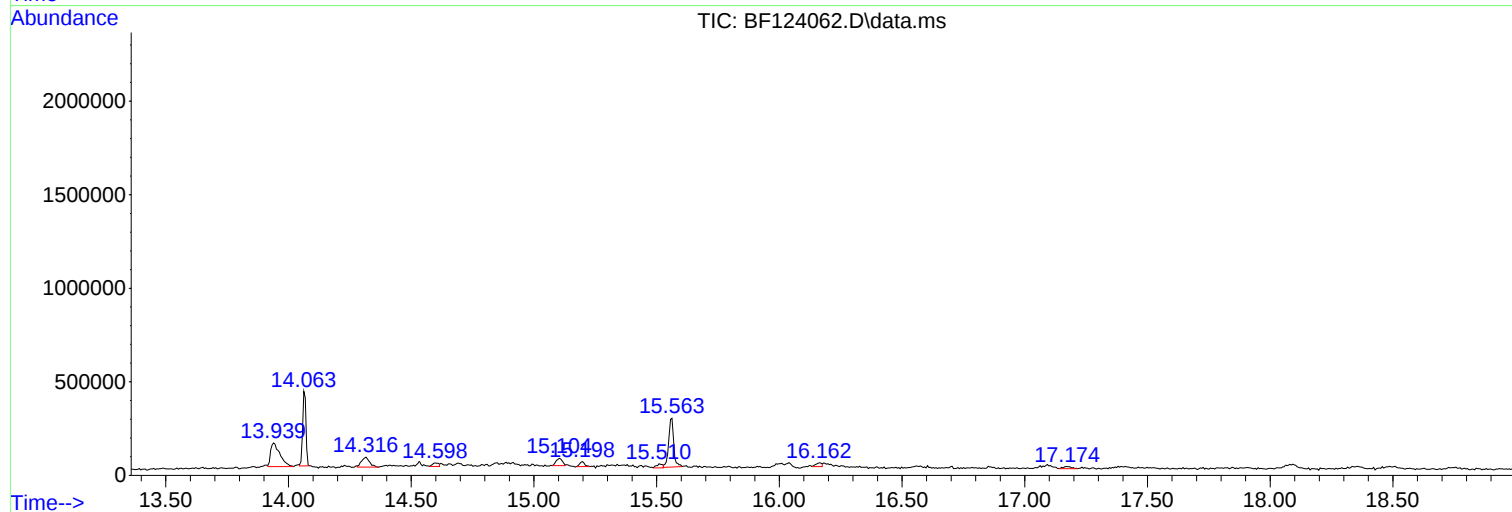
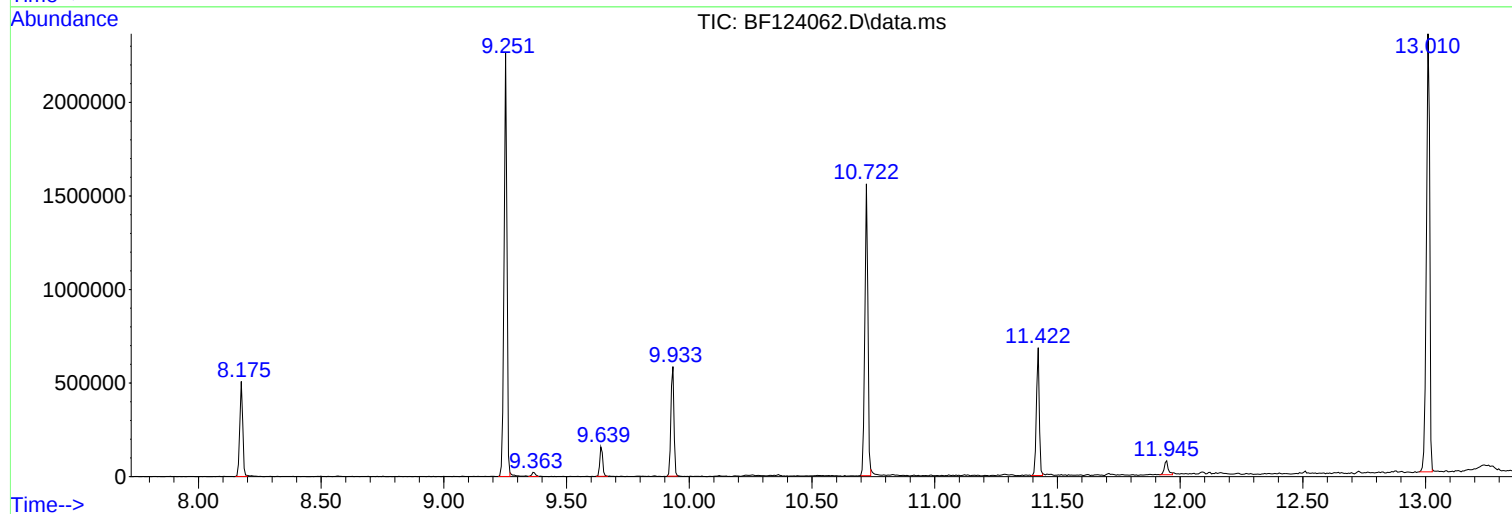
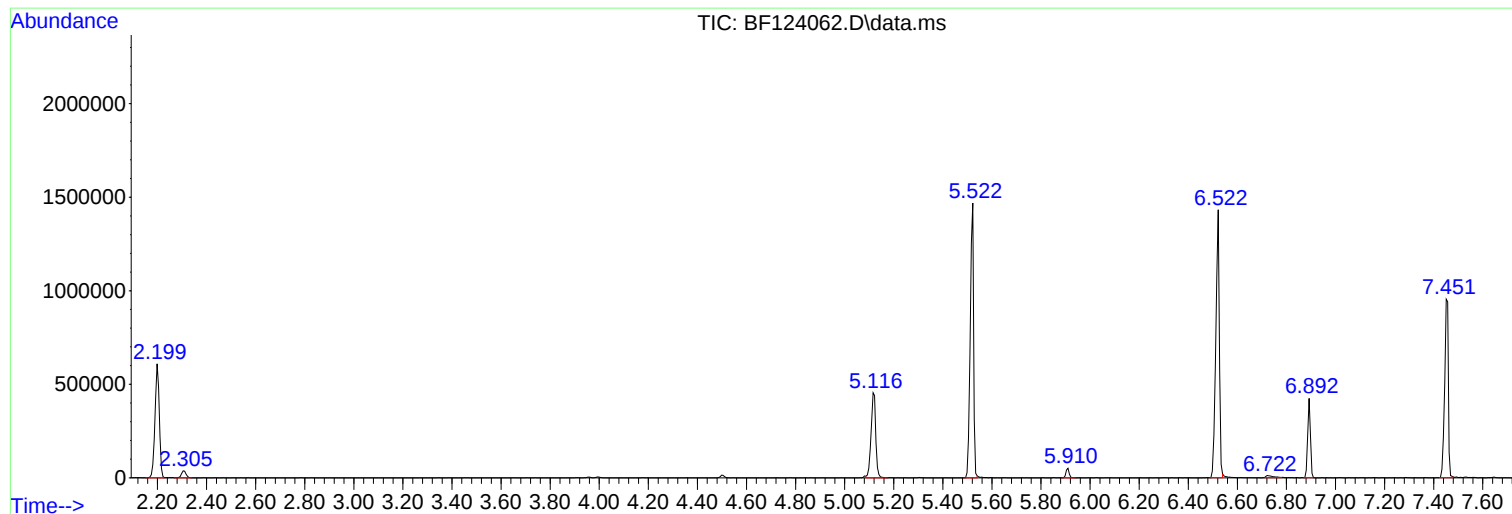
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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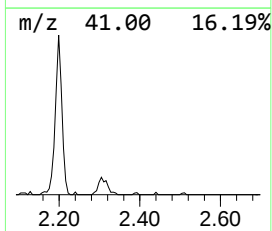
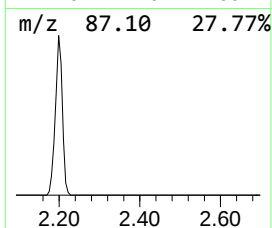
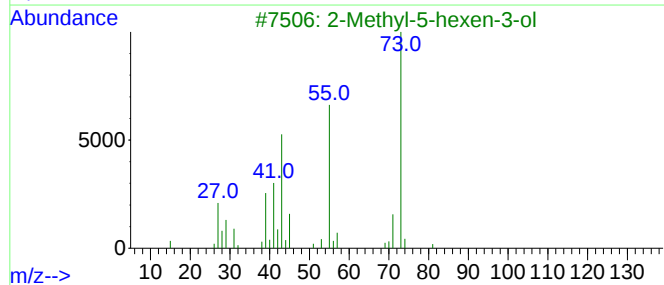
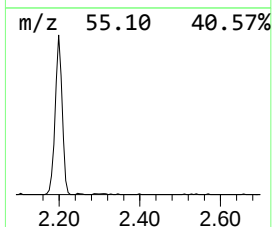
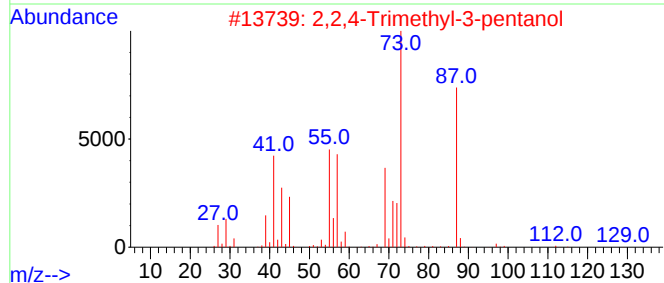
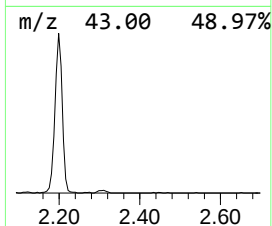
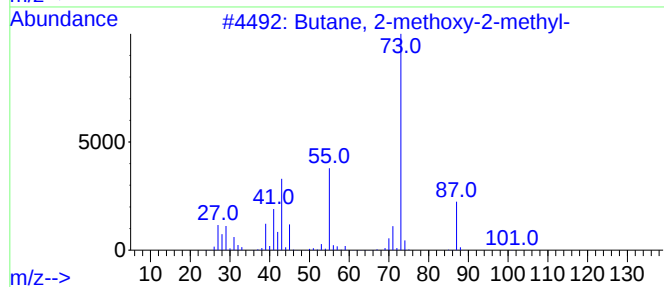
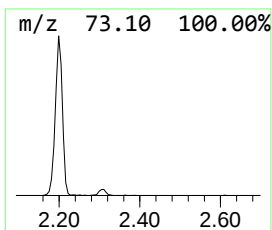
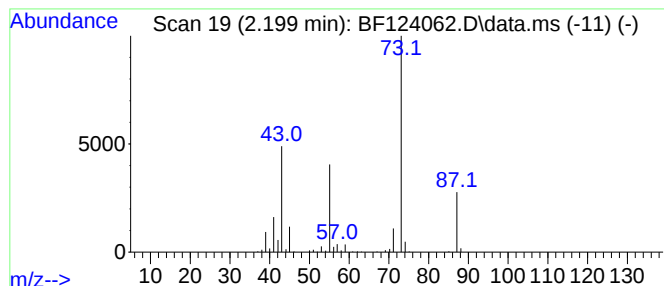
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	45.41 ng	745492	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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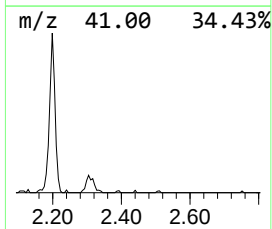
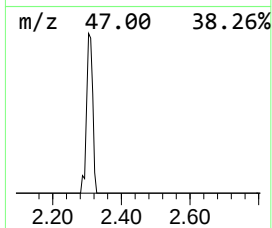
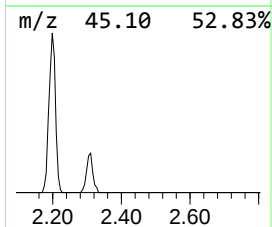
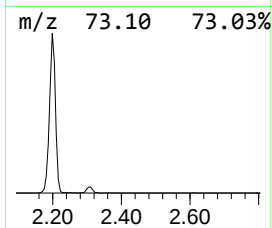
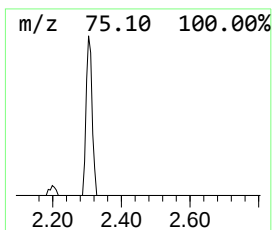
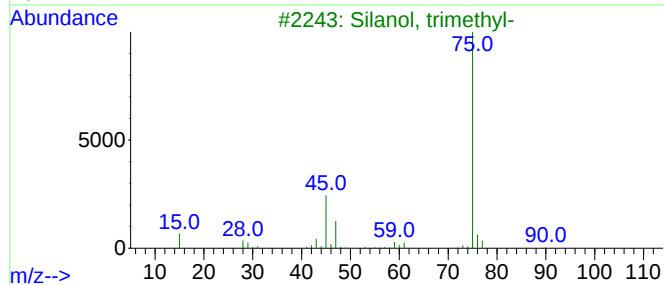
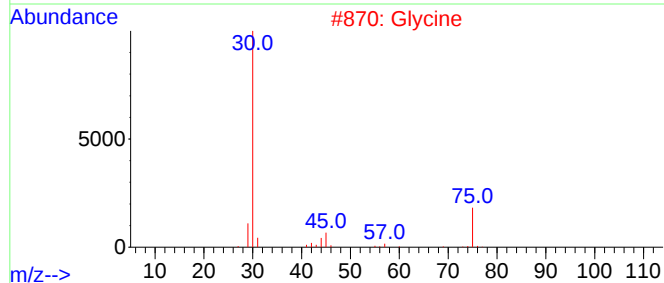
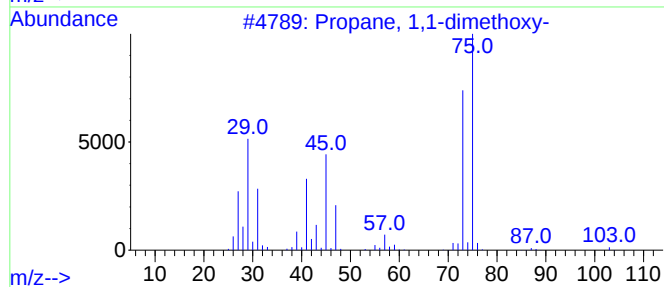
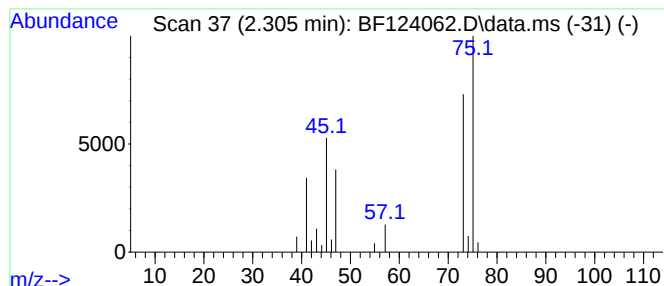
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.305	2.93 ng	48055	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2			Glycine	75	C2H5NO2	000056-40-6	9
3			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
4			Methane, nitroso-	45	CH3NO	000865-40-7	7
5			Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	7



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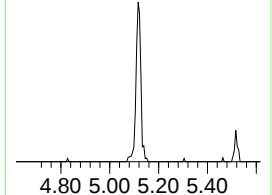
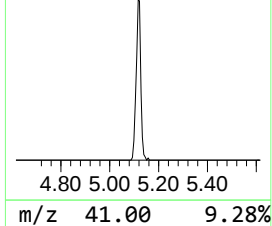
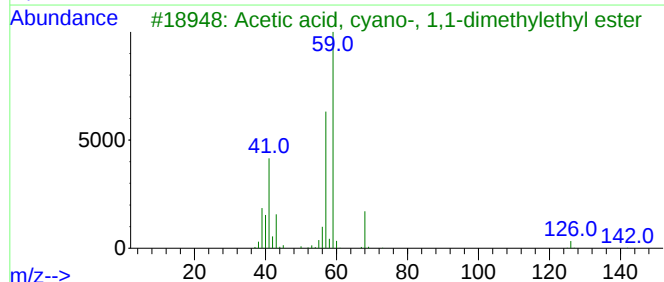
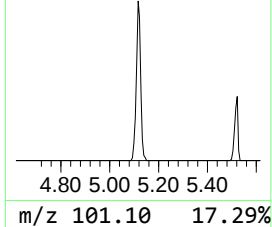
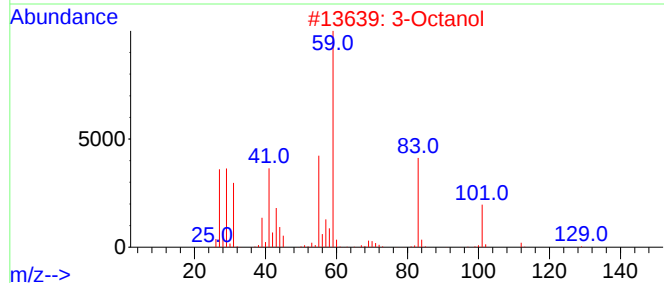
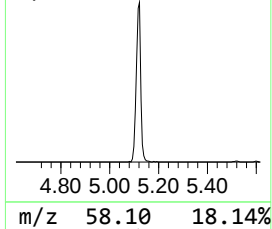
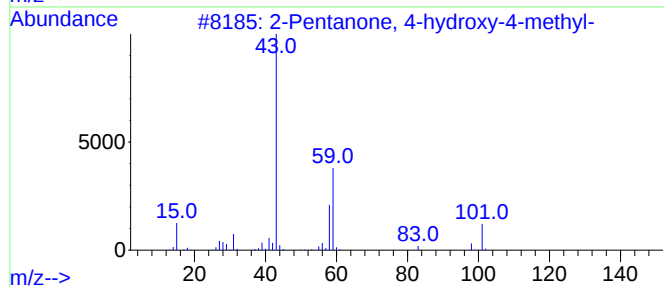
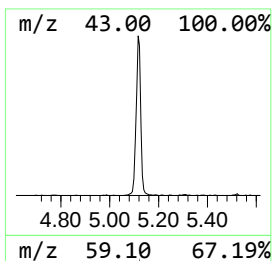
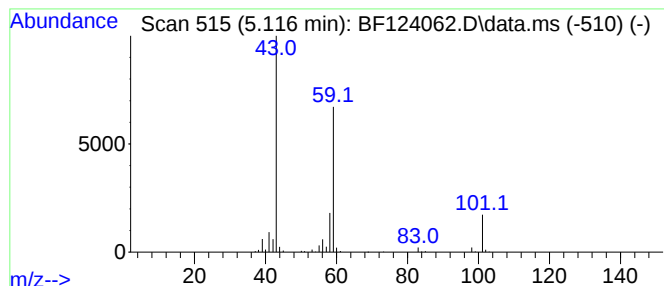
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	36.41 ng	597737	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Octanol	130	C8H18O	000589-98-0	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			Acetone	58	C3H6O	000067-64-1	12



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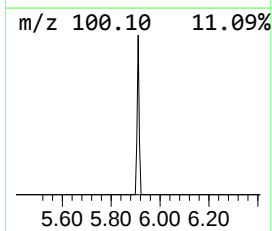
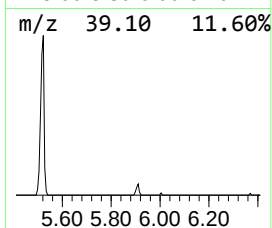
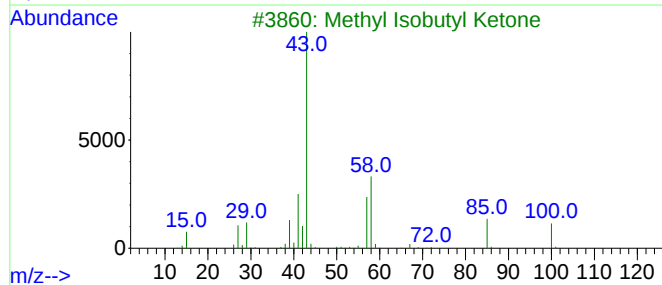
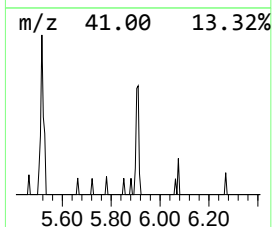
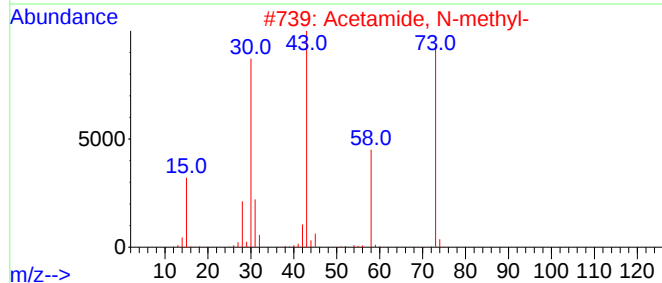
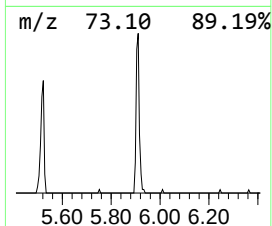
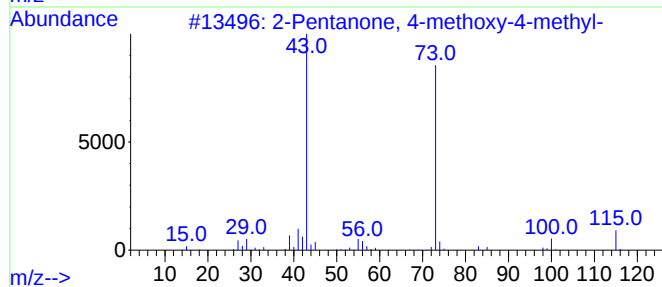
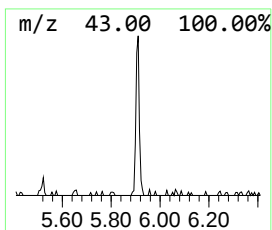
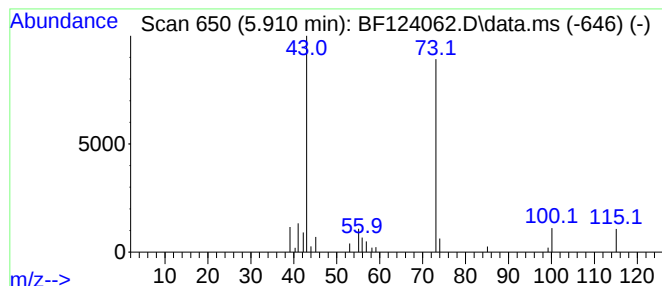
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.910	2.83 ng	46527	1,4-Dichlorobenzene-d4	6.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	52
3		Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	25
4		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	25
5		2-Propanone, oxime	73	C3H7NO	000127-06-0	16



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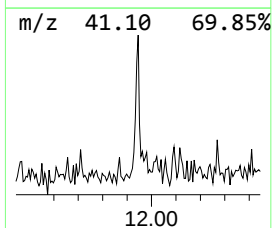
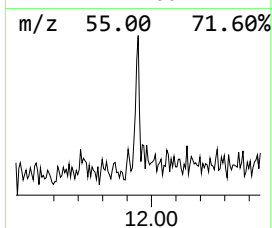
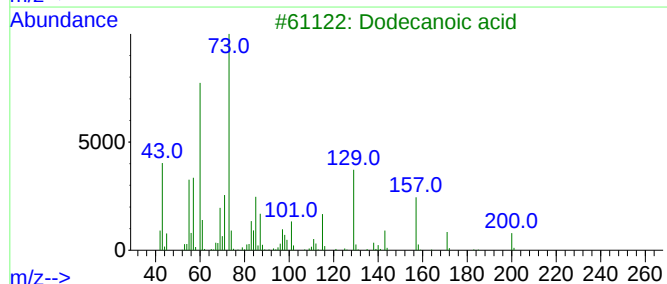
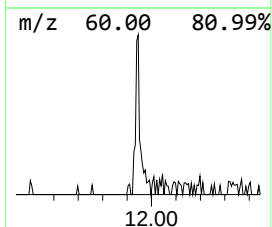
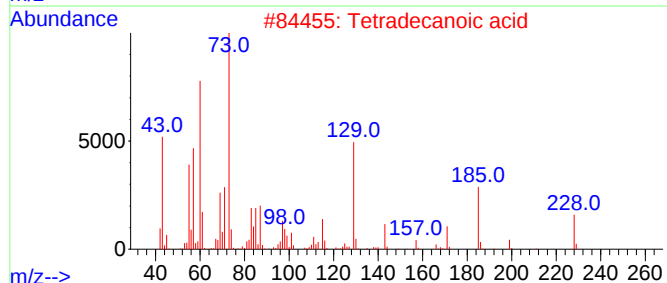
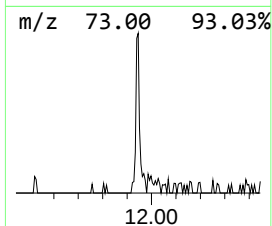
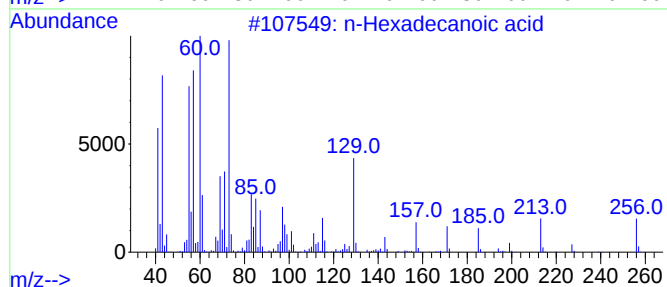
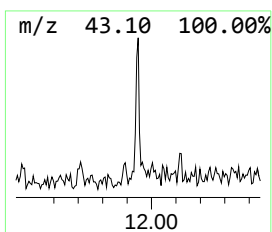
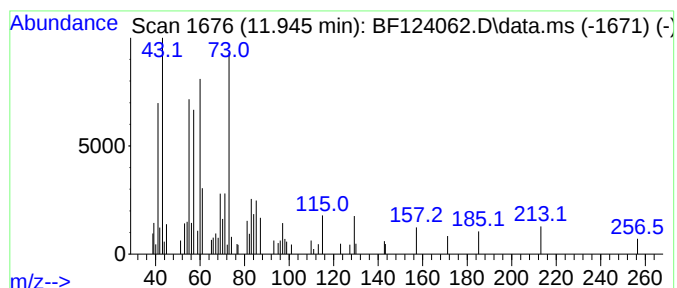
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	3.04 ng	84249	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
3			Dodecanoic acid	200	C12H24O2	000143-07-7	59
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53



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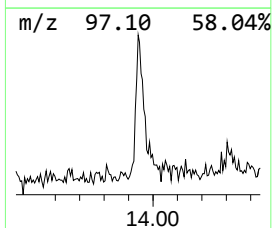
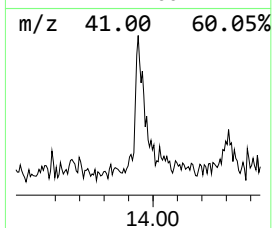
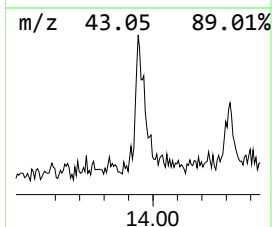
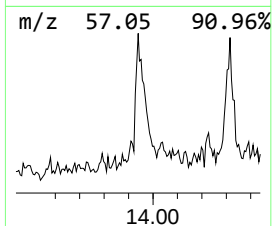
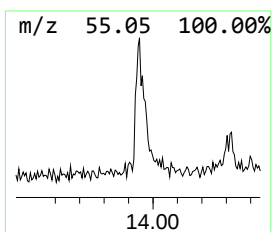
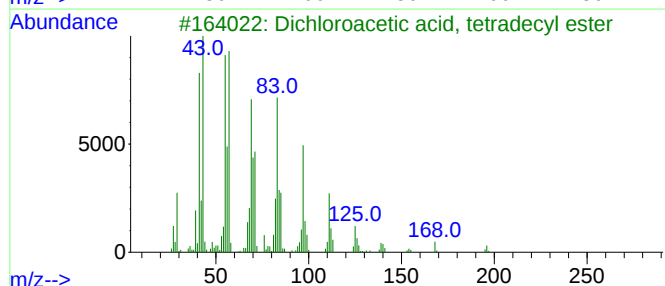
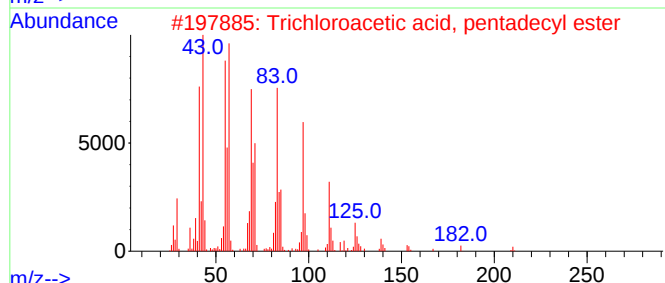
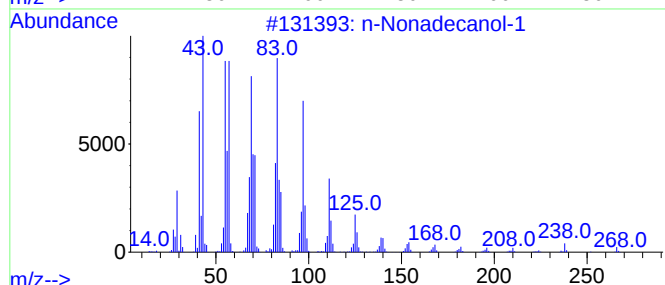
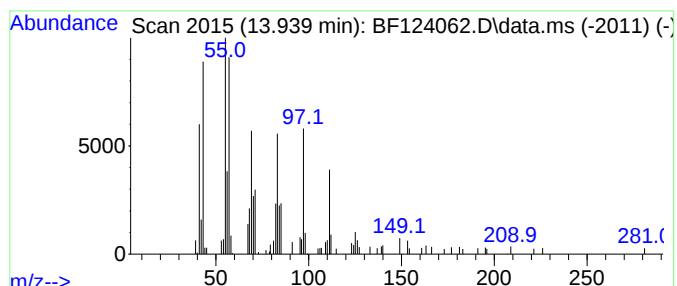
Instrument :
BNA_F
ClientSampleId :
1-5-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.939	17.70 ng	327849	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	80
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	76
3	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	68
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	68
5	17-Pentatriacontene	491	C35H70	006971-40-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124062.D
Acq On : 26 May 2021 13:32
Operator : JU/CG
Sample : M2516-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

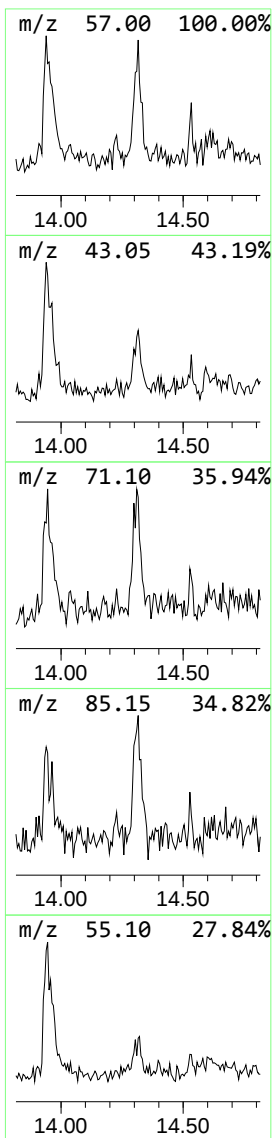
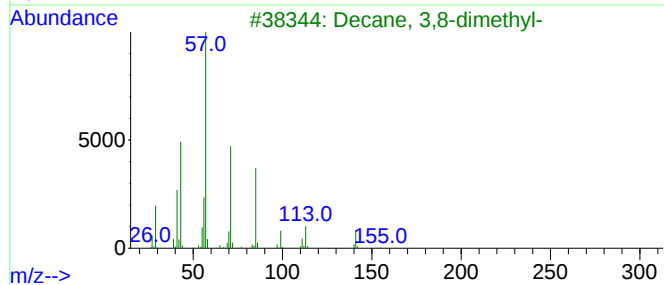
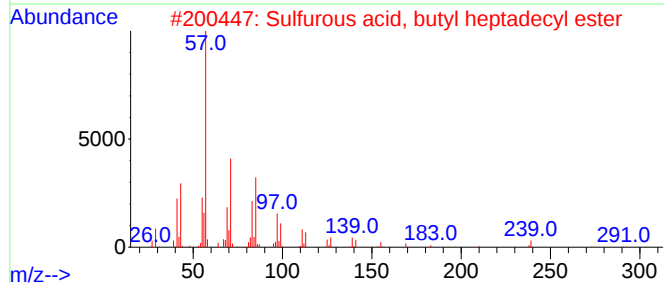
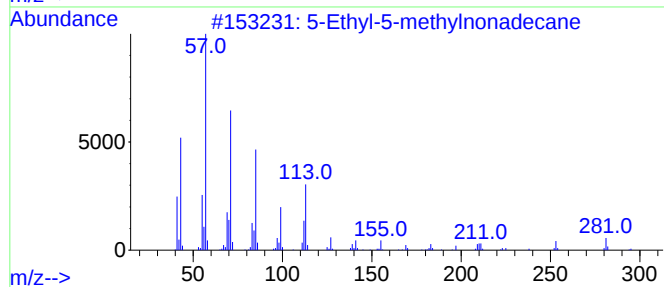
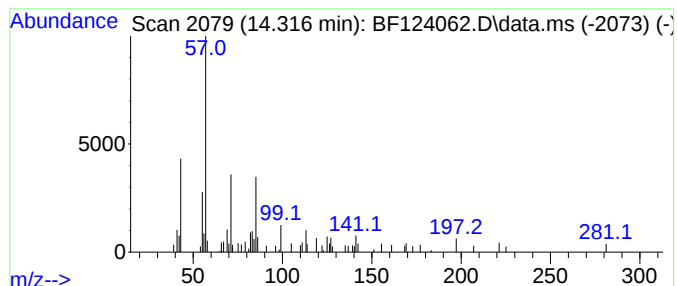
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Ethyl-5-methylnonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.316	6.34 ng	117534	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	64
2	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	59
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	59
4	Pentacosane	352	C25H52	000629-99-2	58
5	Hentriacontane	437	C31H64	000630-04-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124062.D
Acq On : 26 May 2021 13:32
Operator : JU/CG
Sample : M2516-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

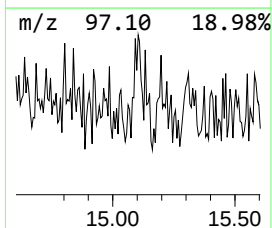
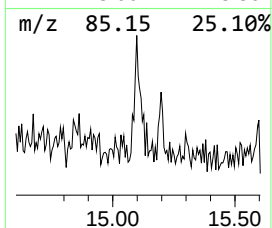
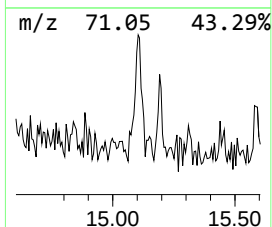
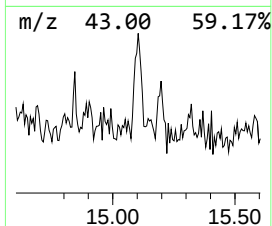
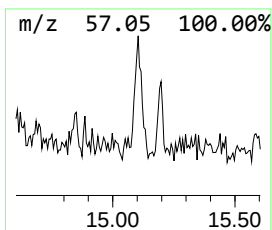
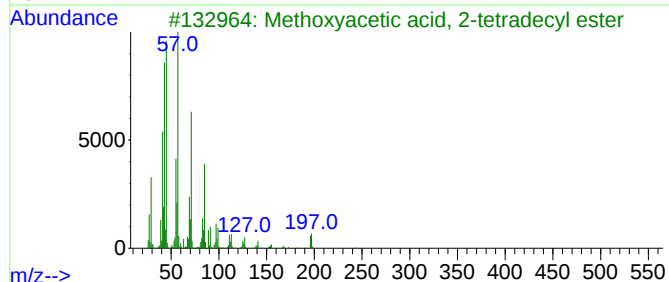
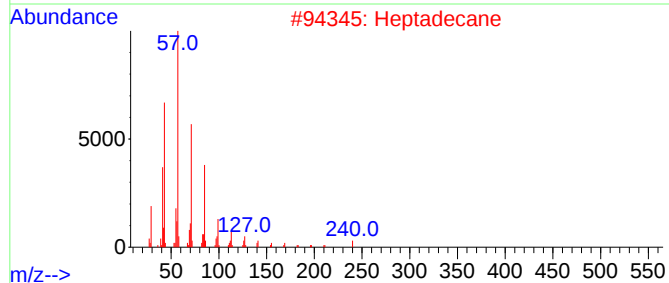
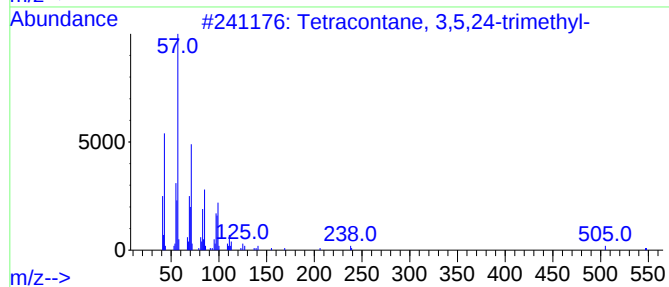
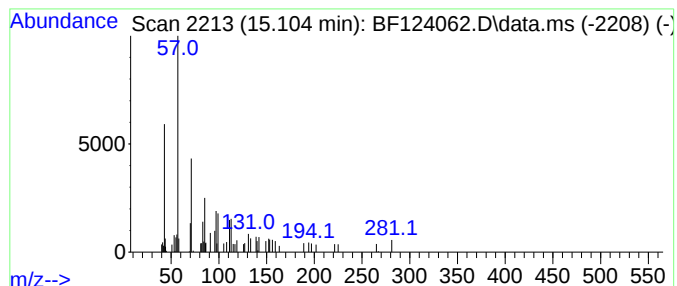
Instrument :
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ClientSampled :
1-5-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracontane, 3,5,24-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.104	3.71 ng	69613	Perylene-d12	15.563	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	53
2	Heptadecane	240	C17H36	000629-78-7	50
3	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	50
4	Heptacosane	380	C27H56	000593-49-7	50
5	Hentriacontane	437	C31H64	000630-04-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124062.D
Acq On : 26 May 2021 13:32
Operator : JU/CG
Sample : M2516-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-5-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.199	45.4	ng	745492	1	6.892	328318	20.0
Propane, 1,1-di...	2.305	2.9	ng	48055	1	6.892	328318	20.0
2-Pentanone, 4-...	5.116	36.4	ng	597737	1	6.892	328318	20.0
2-Pentanone, 4-...	5.910	2.8	ng	46527	1	6.892	328318	20.0
n-Hexadecanoic ...	11.945	3.0	ng	84249	4	11.422	554500	20.0
n-Nonadecanol-1	13.939	17.7	ng	327849	5	14.063	370523	20.0
5-Ethyl-5-methy...	14.316	6.3	ng	117534	5	14.063	370523	20.0
Tetracontane, 3...	15.104	3.7	ng	69613	6	15.563	375105	20.0