

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061721\
 Data File : BG049014.D
 Acq On : 17 Jun 2021 15:01
 Operator : CG/JU
 Sample : M2735-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 124027

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-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049014.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.162	15	21	31	rBV	73859	162562	10.74%	1.633%
2	3.238	31	34	39	rVB2	17710	26963	1.78%	0.271%
3	5.194	363	367	372	rBV	12991	21862	1.44%	0.220%
4	5.665	439	447	456	rBV	465781	775480	51.25%	7.791%
5	7.263	711	719	734	rBV	472233	836656	55.30%	8.405%
6	8.109	856	863	872	rBV	137318	235463	15.56%	2.366%
7	9.278	1050	1062	1071	rBV	290802	532229	35.18%	5.347%
8	10.694	1296	1303	1313	rBV	245799	423886	28.02%	4.259%
9	10.935	1337	1344	1351	rVB	175833	319062	21.09%	3.205%
10	13.373	1753	1759	1770	rVB	653427	1002595	66.27%	10.072%
11	13.643	1798	1805	1810	rBV2	34148	55996	3.70%	0.563%
12	13.943	1851	1856	1862	rVB4	18786	28050	1.85%	0.282%
13	14.754	1987	1994	2003	rVB	286208	448210	29.62%	4.503%
14	16.240	2240	2247	2257	rVB	649813	1013684	67.00%	10.184%
15	17.504	2455	2462	2468	rBV	380356	589331	38.95%	5.921%
16	18.162	2565	2574	2580	rBV	42004	59095	3.91%	0.594%
17	18.385	2606	2612	2622	rBV	130536	190975	12.62%	1.919%
18	19.331	2769	2773	2776	rVB	51036	59837	3.95%	0.601%
19	19.460	2788	2795	2799	rBV	35136	42745	2.83%	0.429%
20	19.554	2805	2811	2817	rVB	15273	26520	1.75%	0.266%
21	19.648	2823	2827	2835	rBV2	75311	104154	6.88%	1.046%
22	19.913	2868	2872	2879	rVB2	11766	21934	1.45%	0.220%
23	20.106	2899	2905	2911	rVB	1183200	1512993	100.00%	15.200%
24	20.788	3018	3021	3028	rVB8	13256	18911	1.25%	0.190%
25	21.423	3124	3129	3135	rBV3	71579	120138	7.94%	1.207%
26	21.675	3168	3172	3177	rVB3	17342	28744	1.90%	0.289%
27	21.793	3183	3192	3198	rBV	381675	659510	43.59%	6.626%
28	25.118	3748	3758	3768	rBV3	218209	636226	42.05%	6.392%

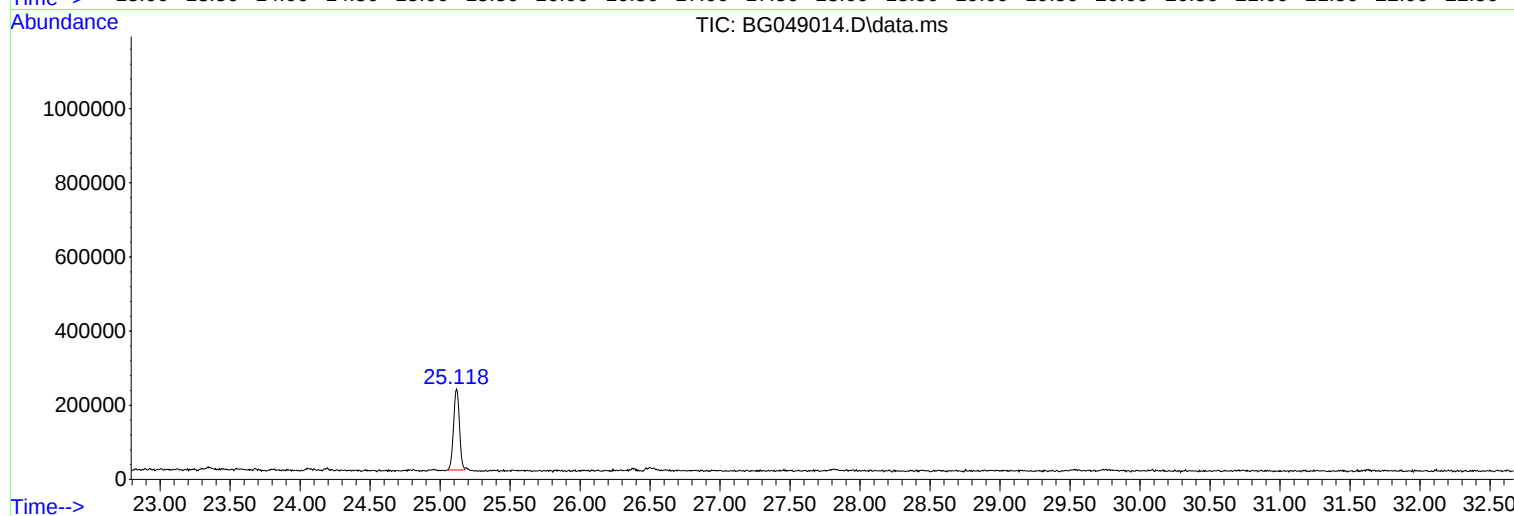
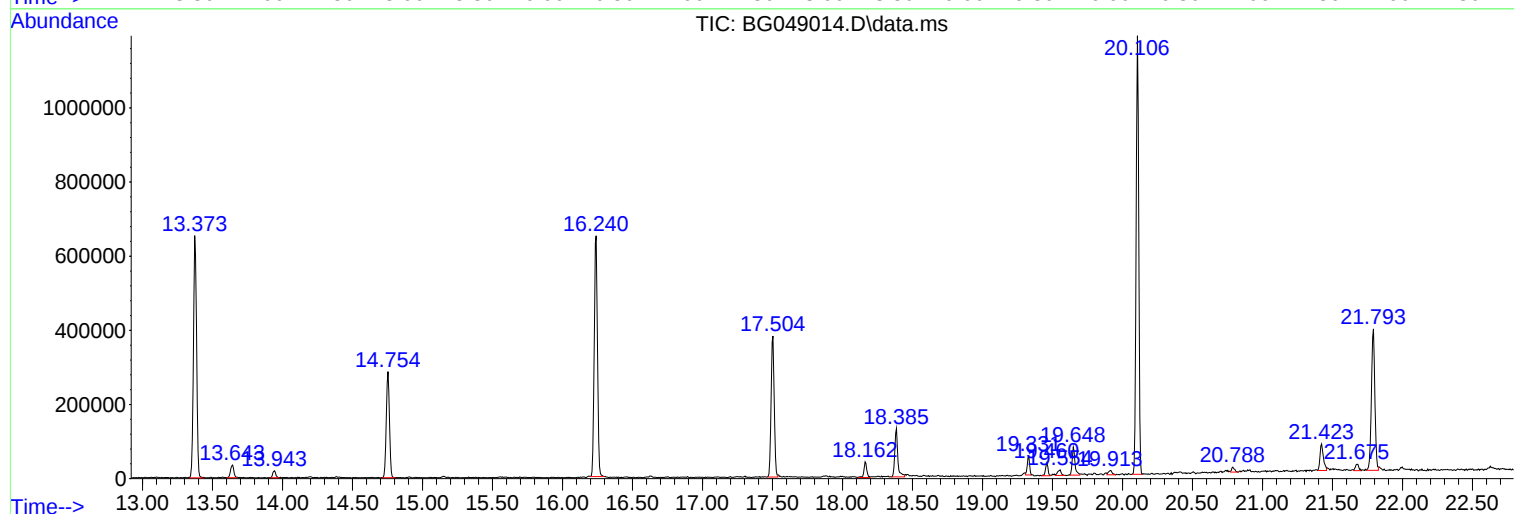
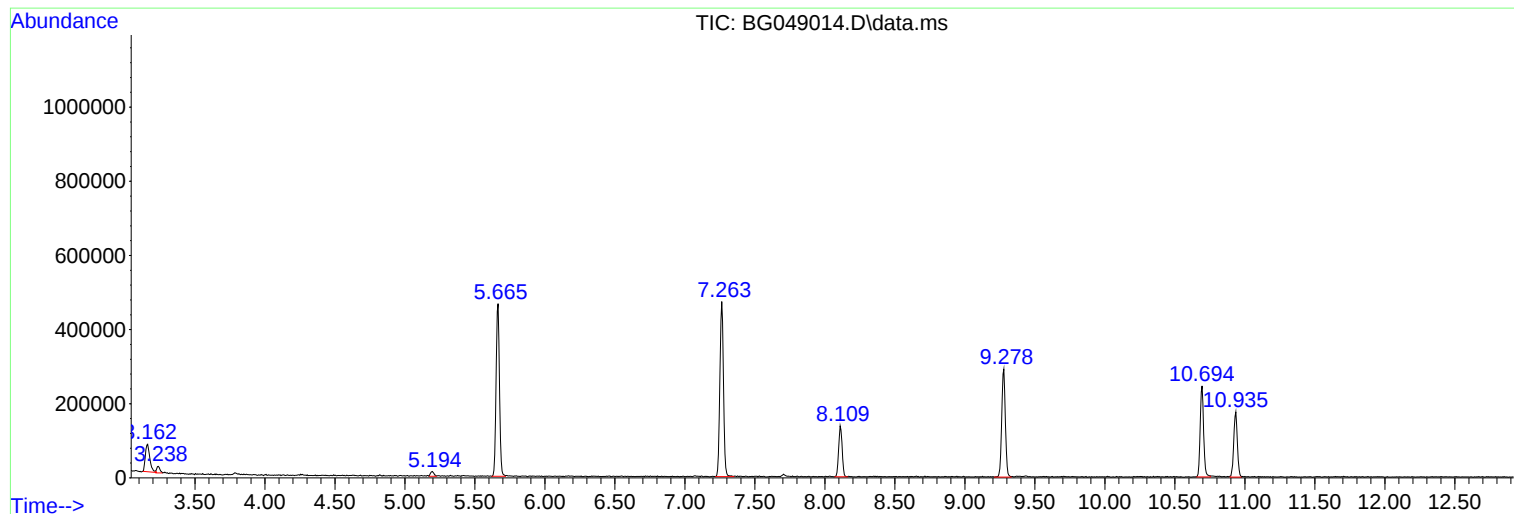
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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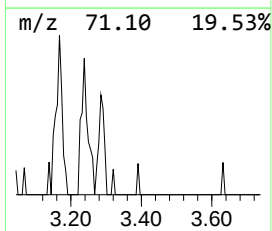
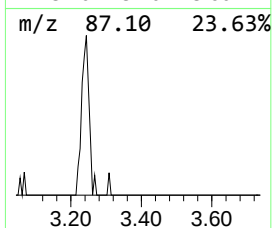
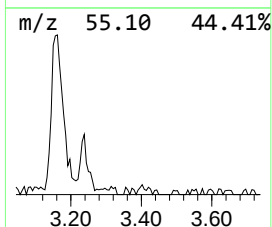
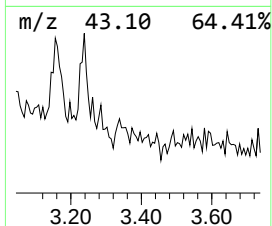
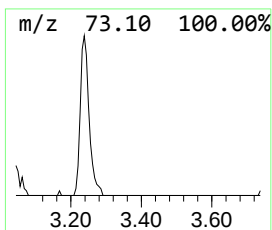
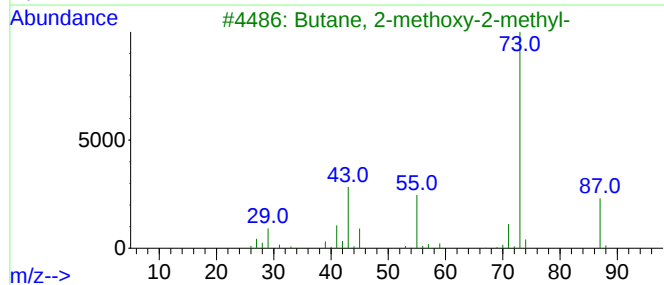
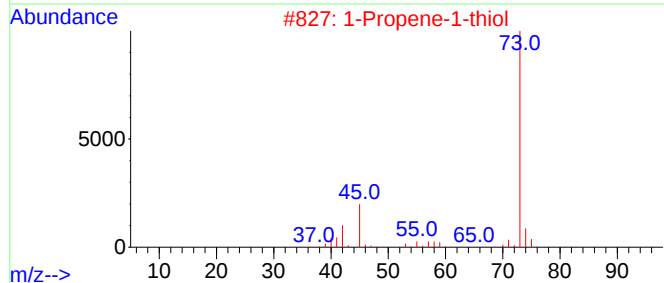
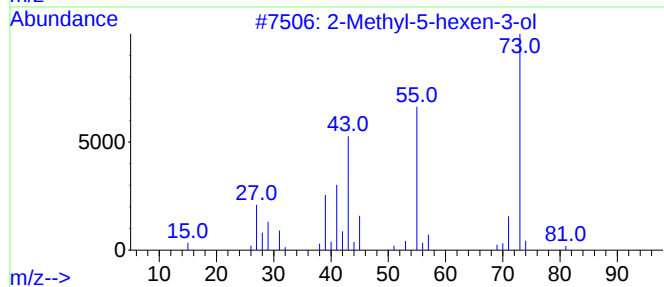
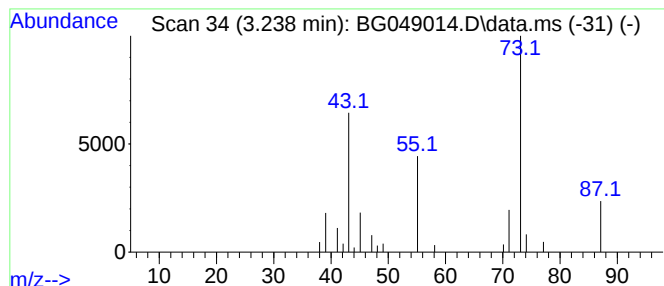
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown3.238 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.238	2.29 ng	26963	1,4-Dichlorobenzene-d4	8.115

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
2		1-Propene-1-thiol	74	C3H6S	000925-89-3	9
3		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
4		Ethyl formate	74	C3H6O2	000109-94-4	7
5		Pyrrolidine	71	C4H9N	000123-75-1	5



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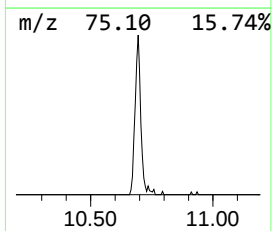
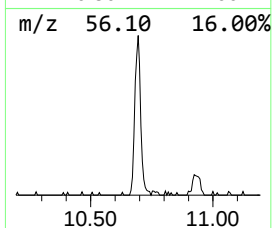
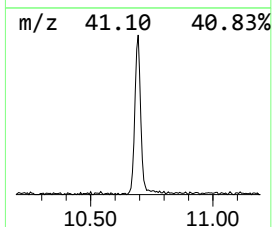
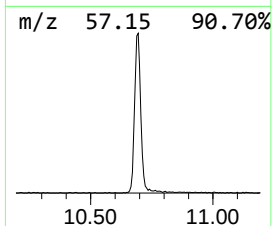
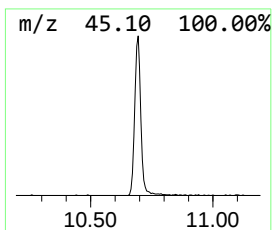
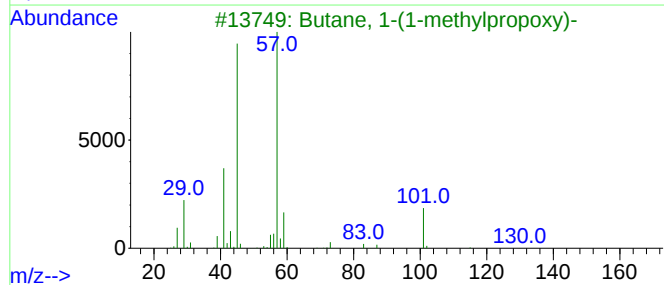
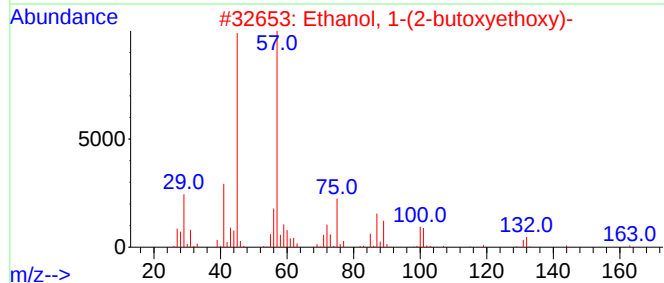
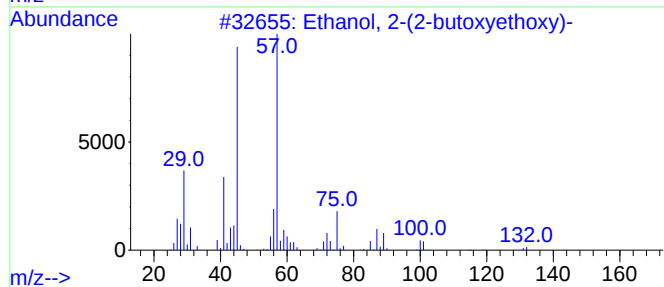
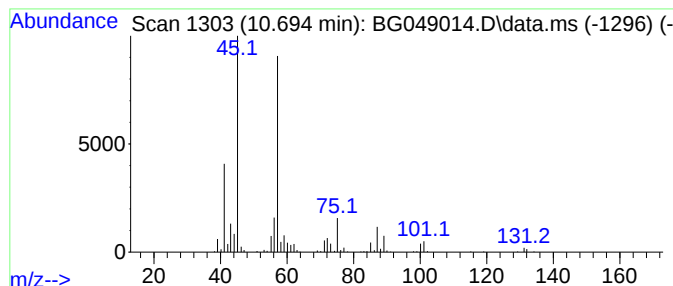
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.694	26.57 ng	423886	Naphthalene-d8	10.935

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4			Di-sec-butyl ether	130	C8H18O	006863-58-7	53
5			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50



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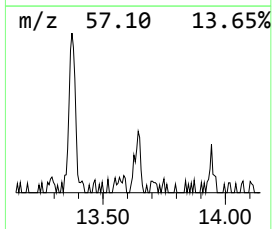
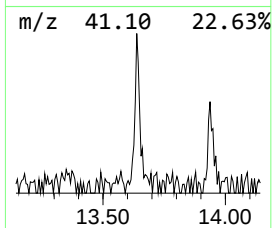
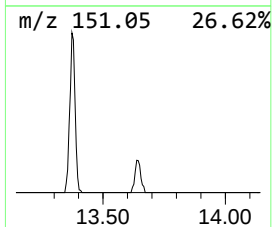
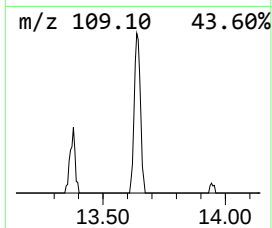
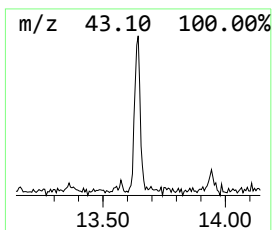
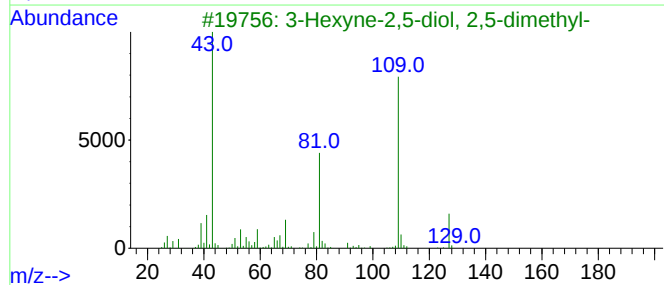
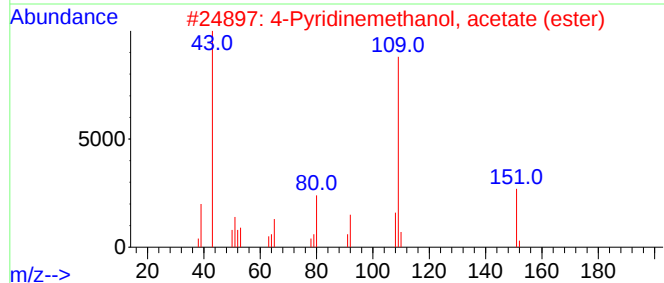
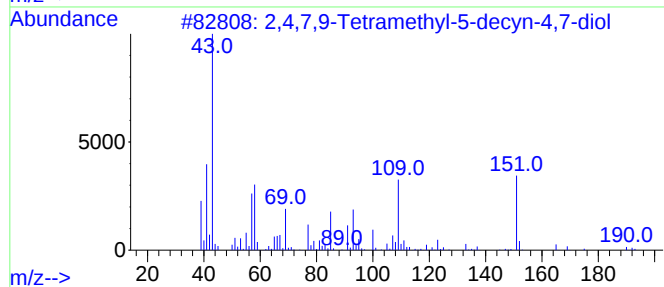
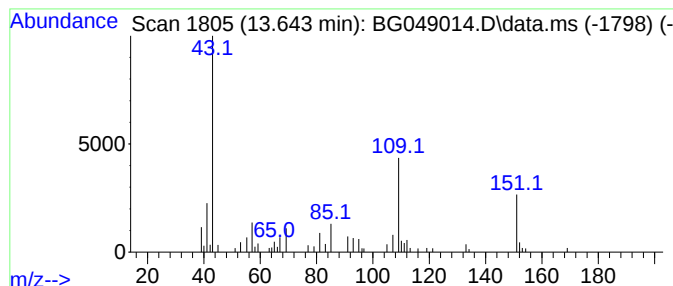
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown13.643 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.643	2.50 ng	55996	Acenaphthene-d10	14.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	40		
2	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	25		
3	3-Hexyne-2,5-diol, 2,5-dimethyl-	142	C8H14O2	000142-30-3	12		
4	Di(n-hexyl)sulfone	234	C12H26O2S	016823-61-3	10		
5	Geranyl acetate, 2,3-epoxy-	212	C12H20O3	050727-95-2	9		



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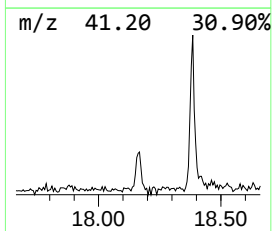
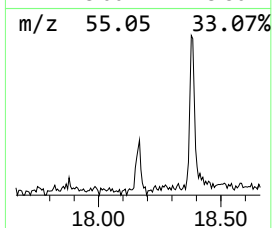
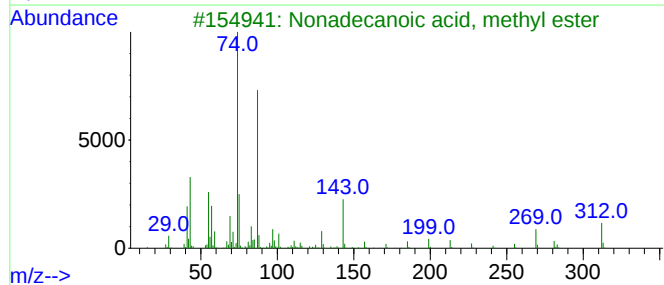
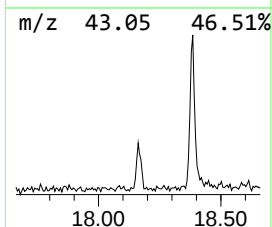
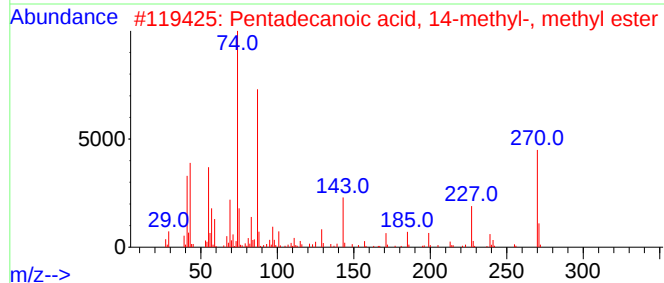
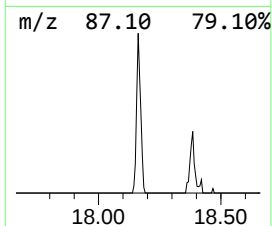
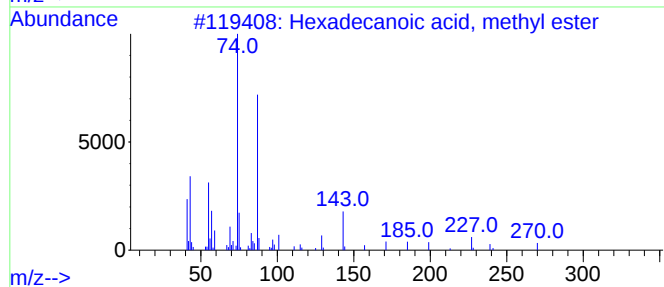
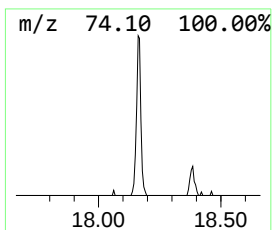
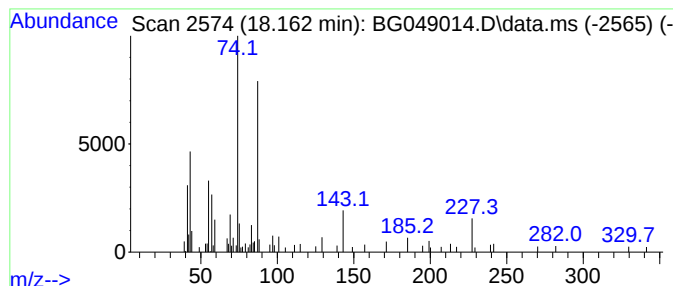
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Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.162	2.01 ng	59095	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	83
4			Methyl stearate	298	C19H38O2	000112-61-8	80
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80



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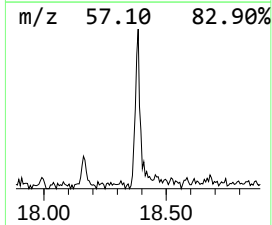
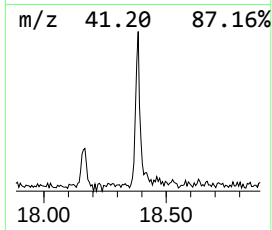
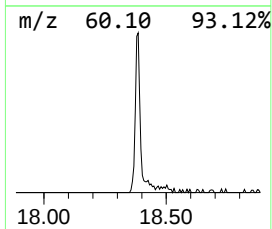
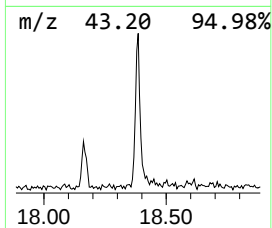
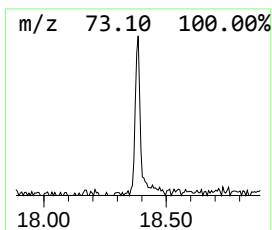
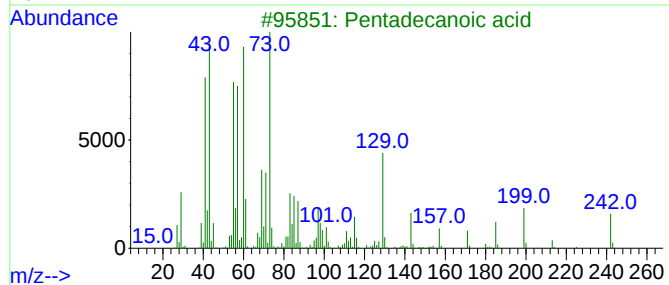
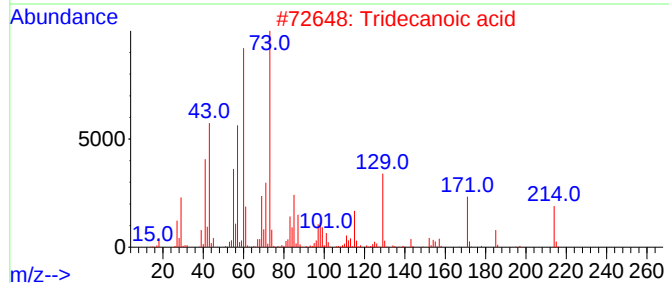
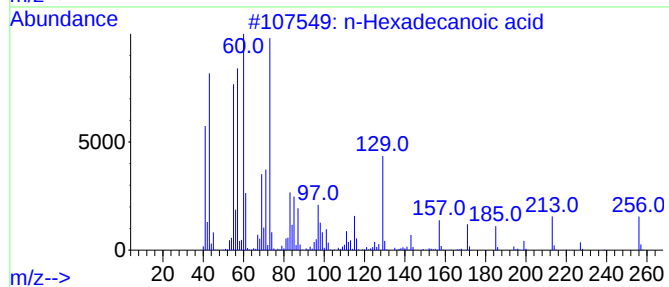
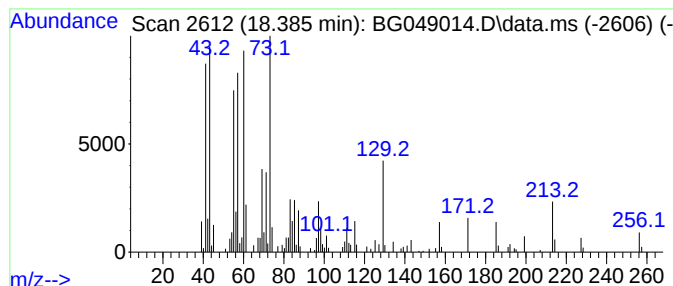
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.385	6.48 ng	190975	Phenanthrene-d10	17.504

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	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Undecanoic acid	186	C11H22O2	000112-37-8	58



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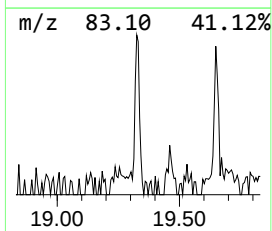
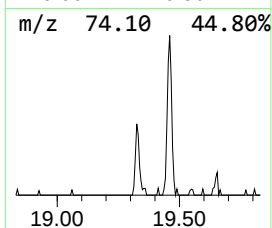
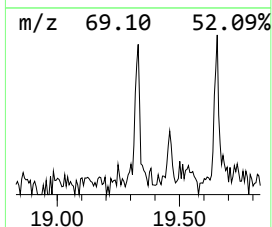
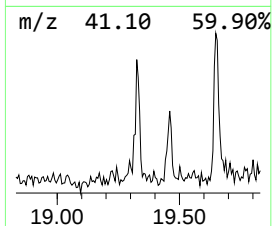
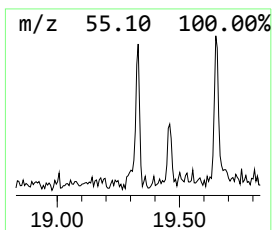
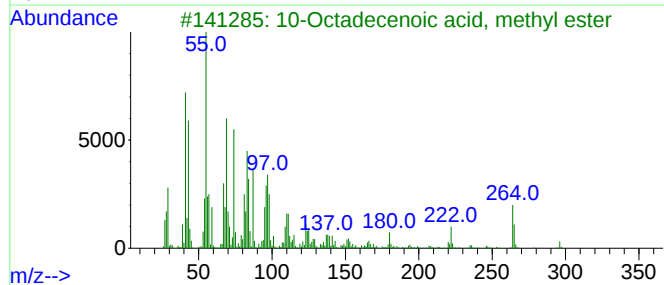
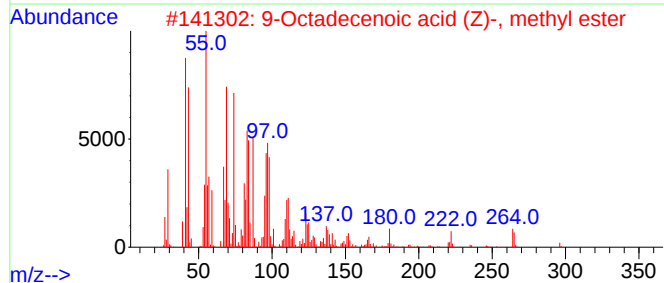
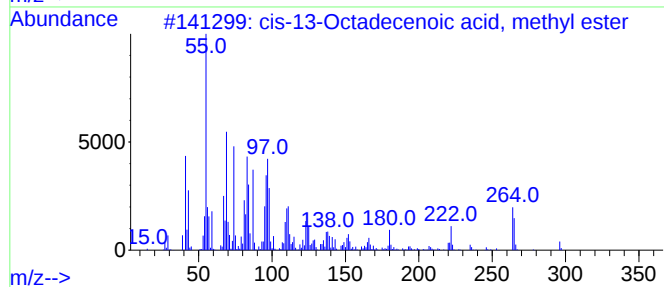
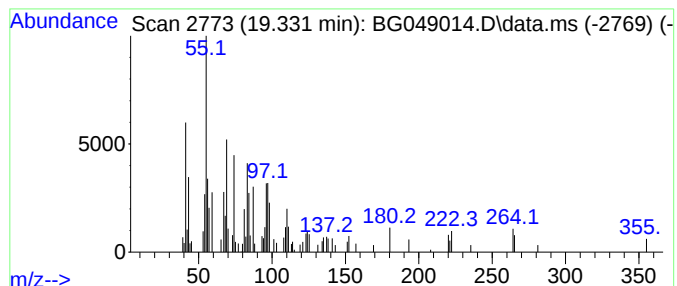
Instrument :
BNA_G
ClientSampleId :
124027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 cis-13-Octadecenoic acid, m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.331	2.03 ng	59837	Phenanthrene-d10	17.504	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	91
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061721\
Data File : BG049014.D
Acq On : 17 Jun 2021 15:01
Operator : CG/JU
Sample : M2735-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124027

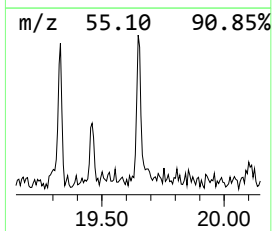
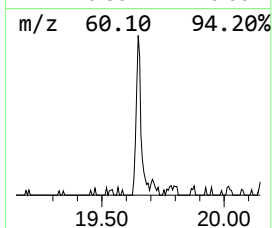
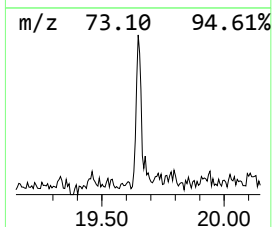
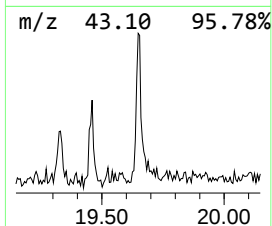
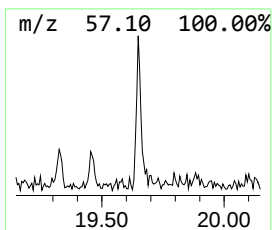
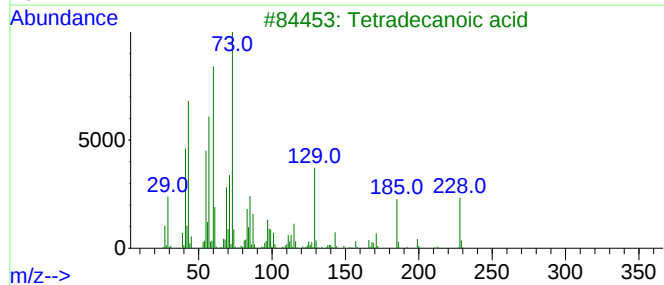
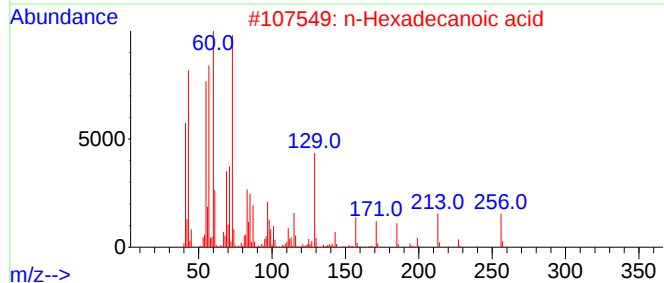
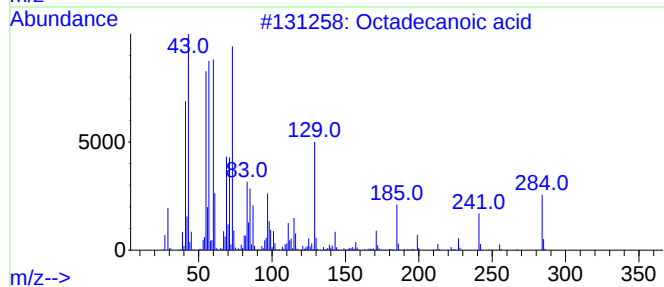
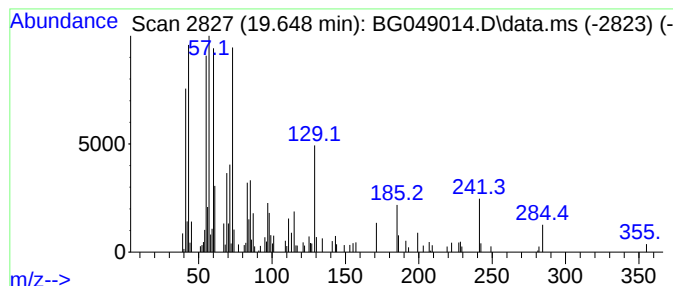
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.648	3.53 ng	104154	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061721\
Data File : BG049014.D
Acq On : 17 Jun 2021 15:01
Operator : CG/JU
Sample : M2735-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124027

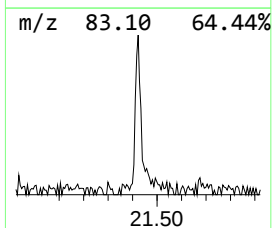
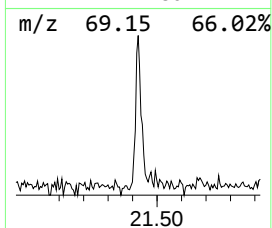
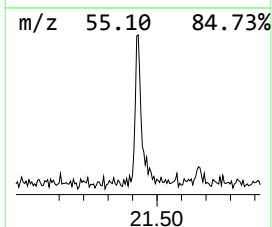
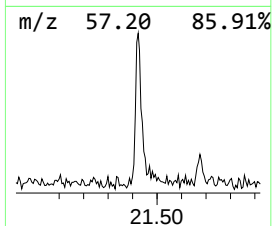
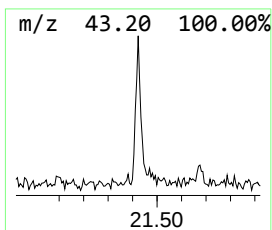
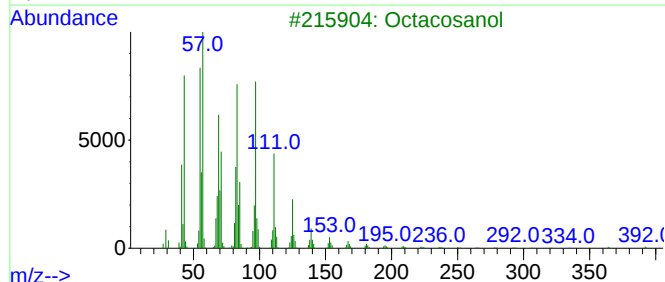
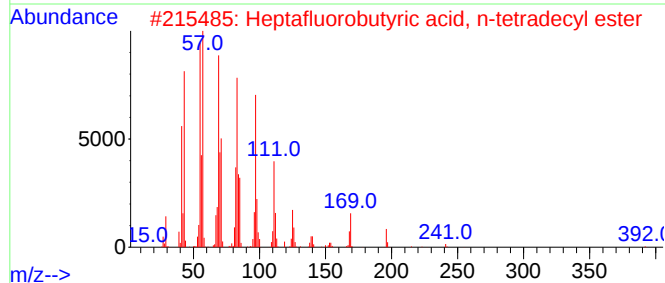
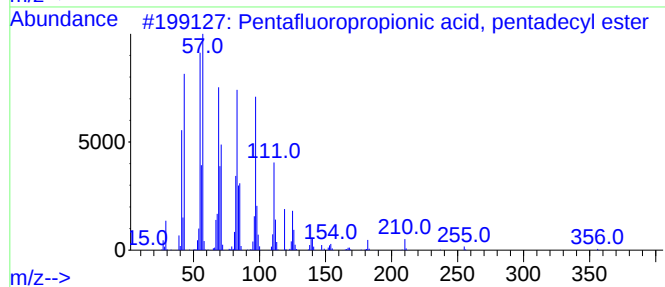
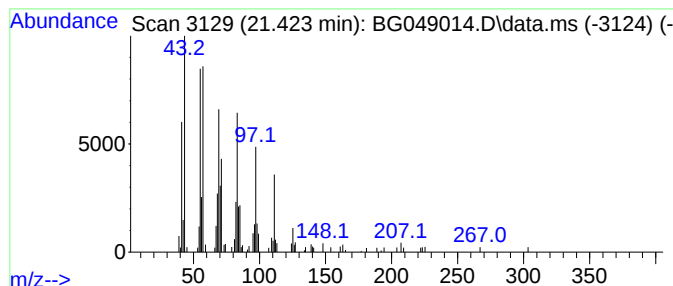
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.422	3.64 ng	120138	Chrysene-d12	21.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3			Octacosanol	410	C28H58O	000557-61-9	91
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061721\
Data File : BG049014.D
Acq On : 17 Jun 2021 15:01
Operator : CG/JU
Sample : M2735-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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
unknown3.238	3.238	2.3	ng	26963	1	8.115	235463	20.0
Ethanol, 2-(2-b...	10.694	26.6	ng	423886	2	10.935	319062	20.0
unknown13.643	13.643	2.5	ng	55996	3	14.754	448210	20.0
Hexadecanoic ac...	18.162	2.0	ng	59095	4	17.504	589331	20.0
n-Hexadecanoic ...	18.385	6.5	ng	190975	4	17.504	589331	20.0
cis-13-Octadece...	19.331	2.0	ng	59837	4	17.504	589331	20.0
Octadecanoic acid	19.648	3.5	ng	104154	4	17.504	589331	20.0
Pentafluoroprop...	21.422	3.6	ng	120138	5	21.793	659510	20.0