

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
 Data File : BG055614.D
 Acq On : 14 Nov 2022 21:29
 Operator : CG/JU
 Sample : N5531-12
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-28A

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-BG110922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055614.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.323	3	6	19	rVB	231159	356942	13.66%	2.220%
2	5.315	339	345	352	rVB	112460	178971	6.85%	1.113%
3	5.791	419	426	435	rBV	792060	1277170	48.87%	7.943%
4	7.401	692	700	710	rBV	813358	1394180	53.34%	8.671%
5	8.264	840	847	855	rBV	189917	321283	12.29%	1.998%
6	9.434	1038	1046	1054	rBV	491670	872002	33.36%	5.423%
7	10.838	1279	1285	1296	rBV	51386	89184	3.41%	0.555%
8	11.091	1321	1328	1337	rBV	259673	481428	18.42%	2.994%
9	13.511	1731	1740	1747	rBV	1322643	2056208	78.67%	12.788%
10	14.886	1966	1974	1981	rBV	421723	667060	25.52%	4.149%
11	15.656	2100	2105	2117	rVB4	10971	28745	1.10%	0.179%
12	16.367	2219	2226	2236	rBV	1074456	1628339	62.30%	10.127%
13	17.624	2434	2440	2446	rBV	509004	782996	29.96%	4.870%
14	17.665	2446	2447	2454	rVB	23593	28599	1.09%	0.178%
15	18.265	2545	2549	2554	rVB3	24694	33047	1.26%	0.206%
16	18.488	2581	2587	2593	rBV2	164655	265778	10.17%	1.653%
17	18.547	2593	2597	2604	rVB2	32389	58399	2.23%	0.363%
18	18.688	2616	2621	2626	rBV2	45875	97847	3.74%	0.609%
19	18.729	2626	2628	2632	rVB	25384	27998	1.07%	0.174%
20	19.399	2738	2742	2749	rBV	57994	126856	4.85%	0.789%
21	19.540	2762	2766	2767	rBV4	24954	30222	1.16%	0.188%
22	19.663	2783	2787	2793	rVB	123480	177882	6.81%	1.106%
23	19.745	2797	2801	2809	rVB3	80402	119277	4.56%	0.742%
24	20.027	2842	2849	2855	rVB	200157	323143	12.36%	2.010%
25	20.092	2857	2860	2867	rVB3	24480	38099	1.46%	0.237%
26	20.215	2875	2881	2886	rBV	2064107	2613577	100.00%	16.254%
27	20.673	2956	2959	2962	rBV	33115	41910	1.60%	0.261%
28	20.814	2979	2983	2986	rBV	50523	67172	2.57%	0.418%
29	20.861	2988	2991	2994	rVB	45164	57537	2.20%	0.358%
30	21.531	3101	3105	3119	rBV2	116747	241910	9.26%	1.504%
31	21.925	3165	3172	3178	rBV2	450389	917289	35.10%	5.705%
32	25.356	3748	3756	3768	rBV2	232359	678147	25.95%	4.218%

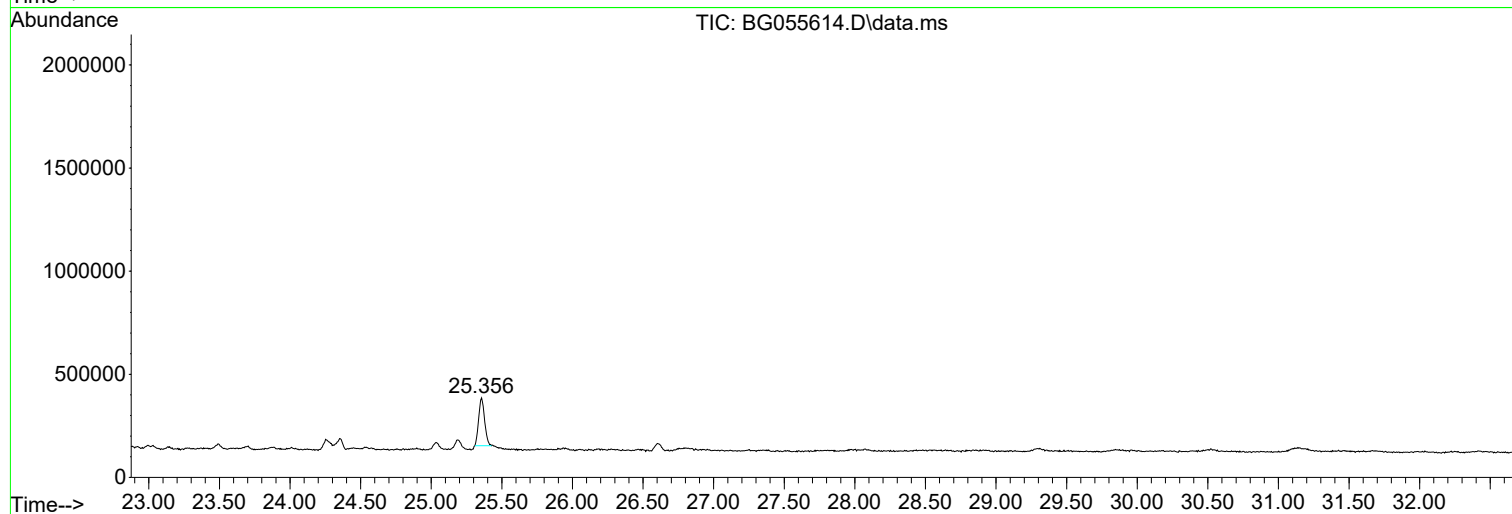
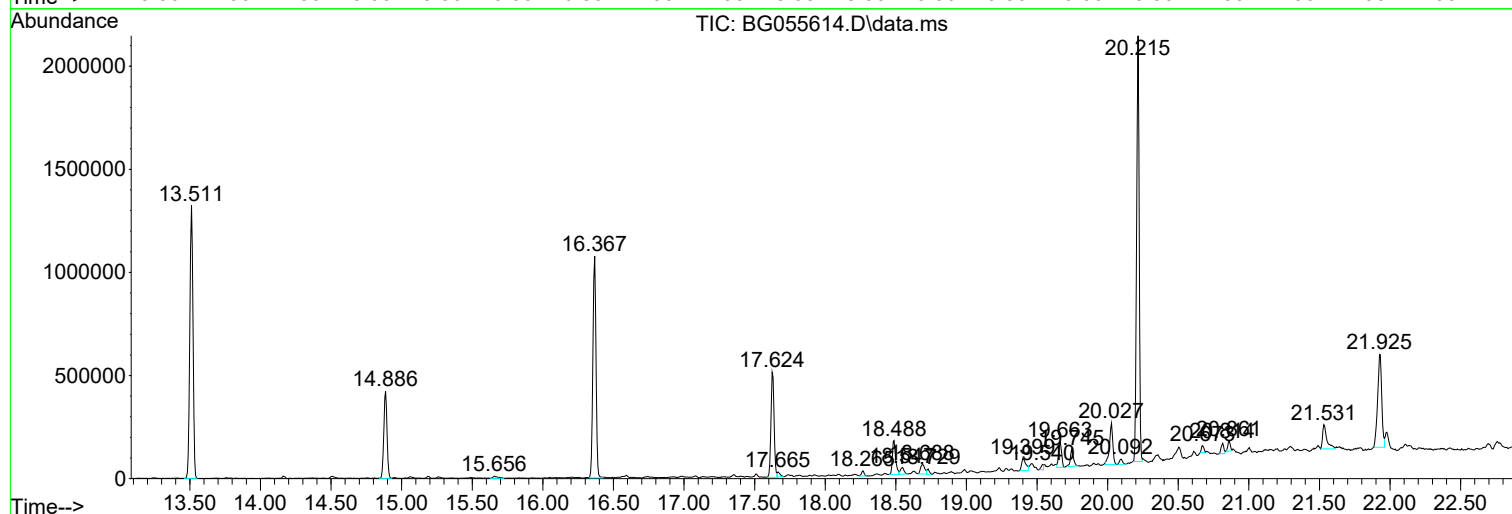
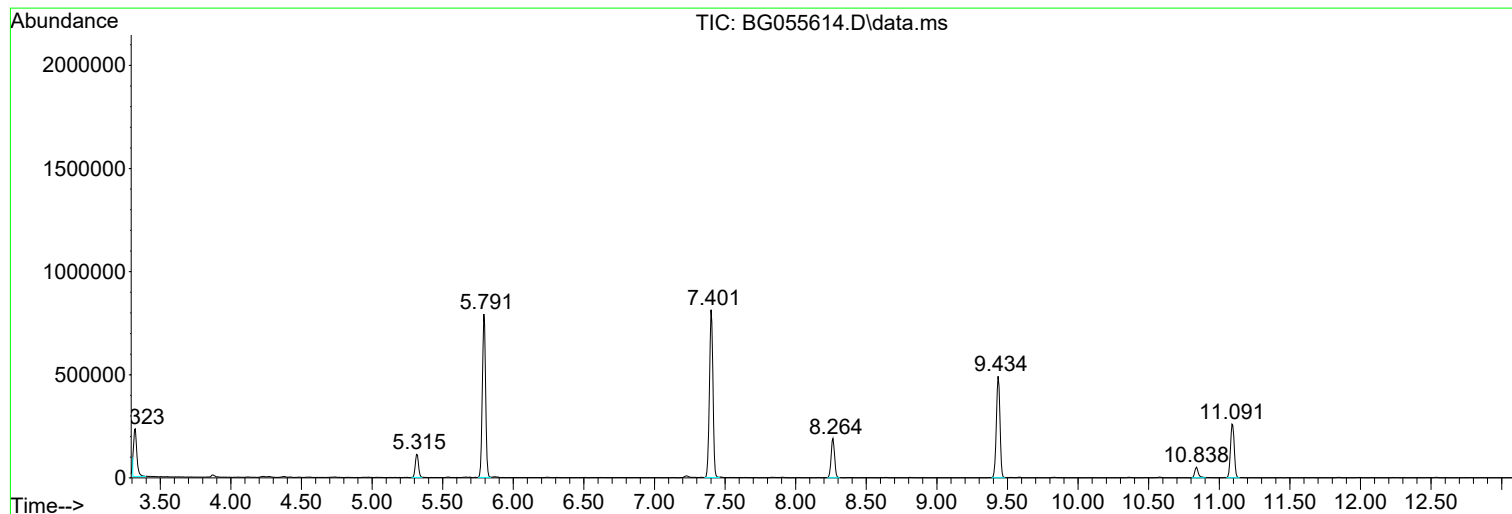
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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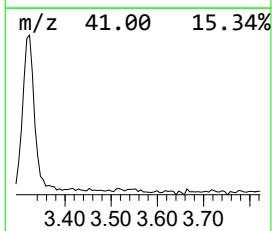
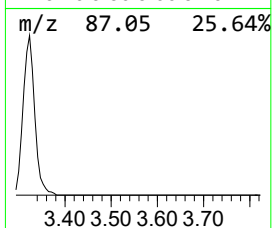
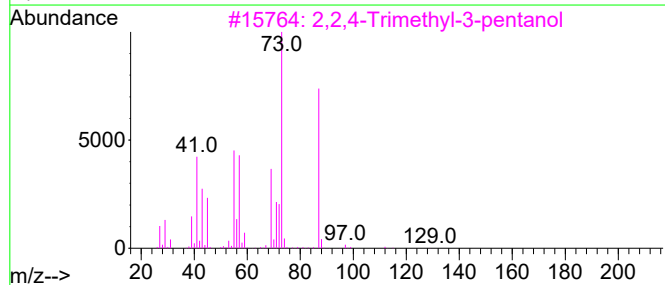
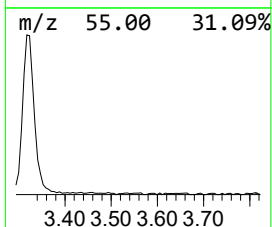
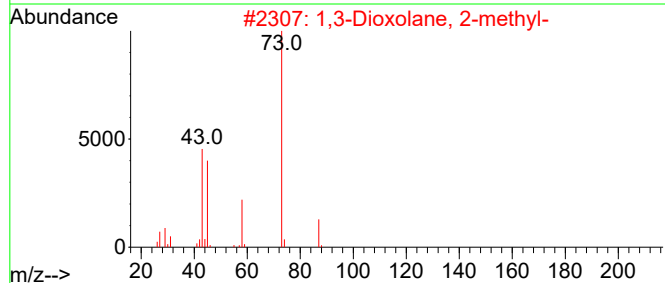
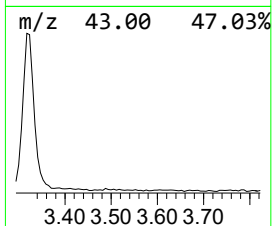
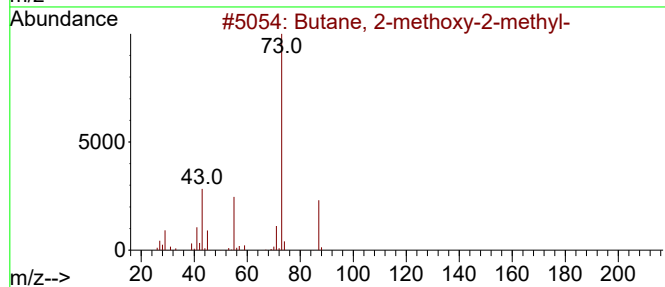
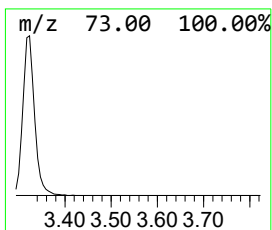
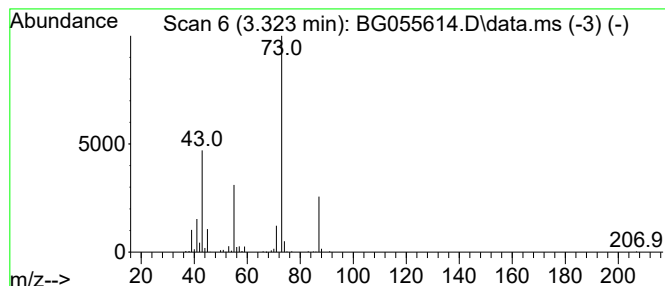
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.323	22.22 ng	356942	1,4-Dichlorobenzene-d4	8.264

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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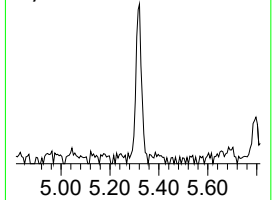
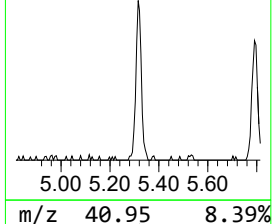
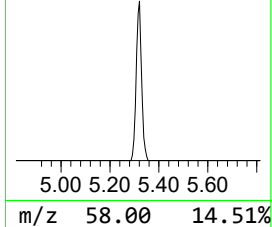
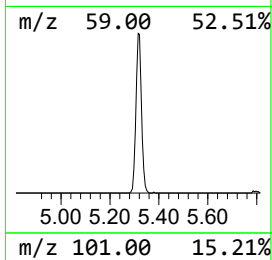
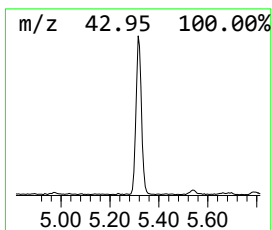
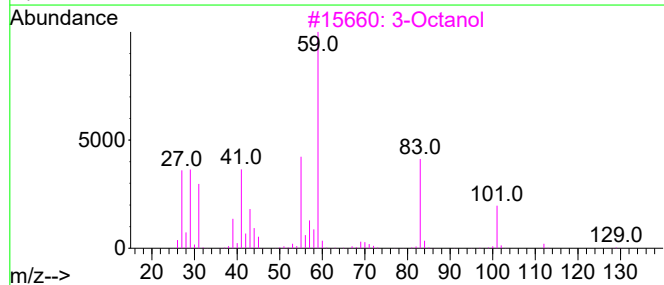
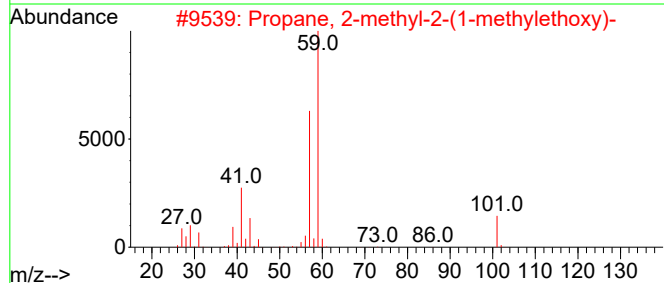
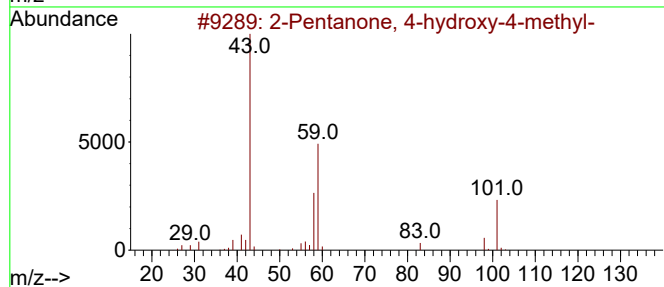
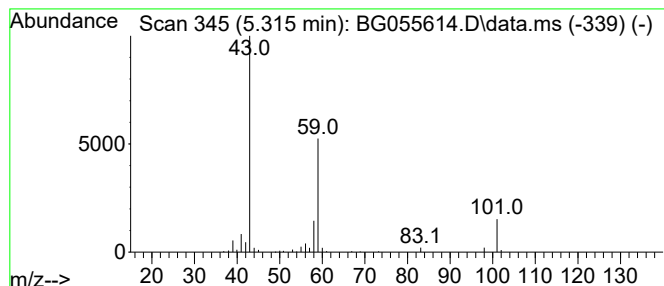
Instrument :
BNA_G
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.315	11.14 ng	178971	1,4-Dichlorobenzene-d4			8.264
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	36
3	3-Octanol		130	C8H18O	000589-98-0	33
4	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	28
5	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28



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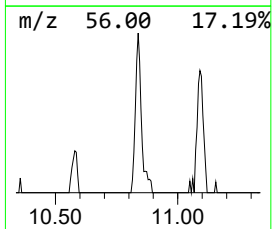
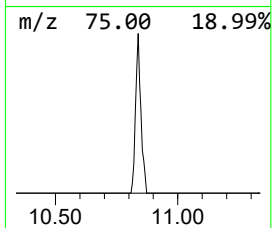
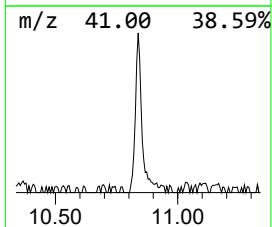
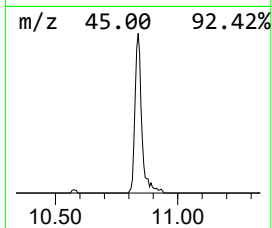
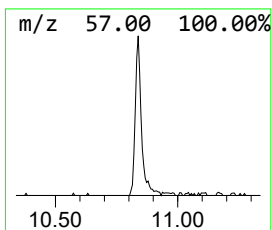
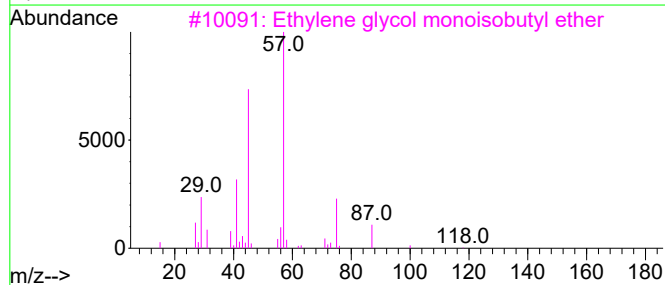
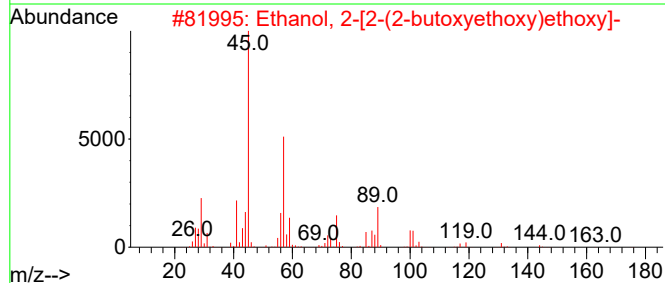
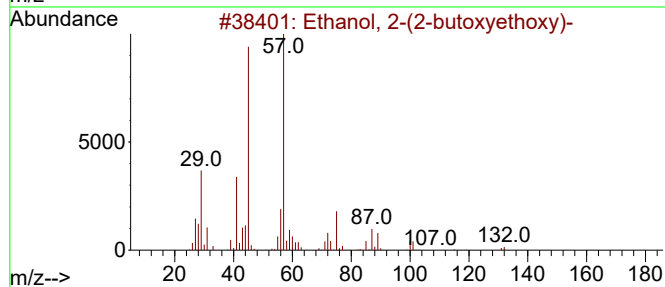
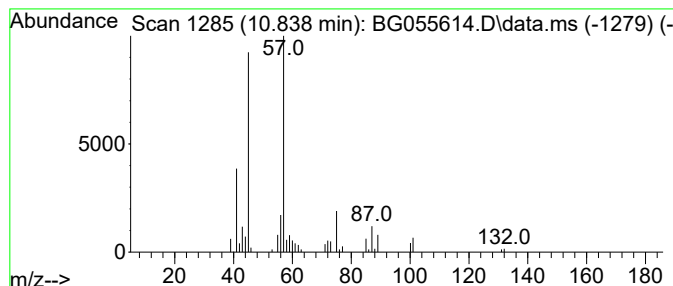
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.838	3.70 ng	89184	Naphthalene-d8	11.091

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	72
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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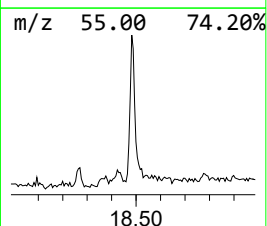
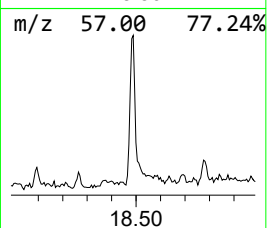
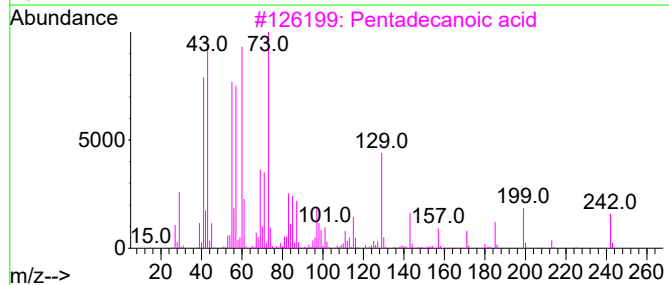
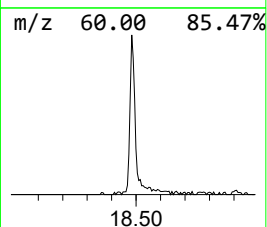
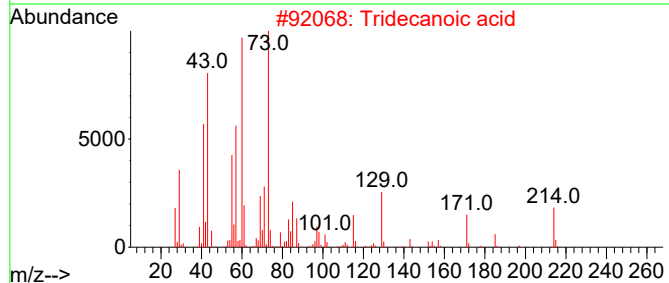
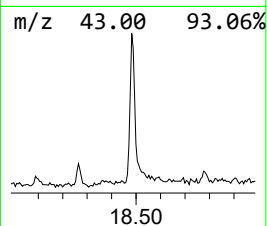
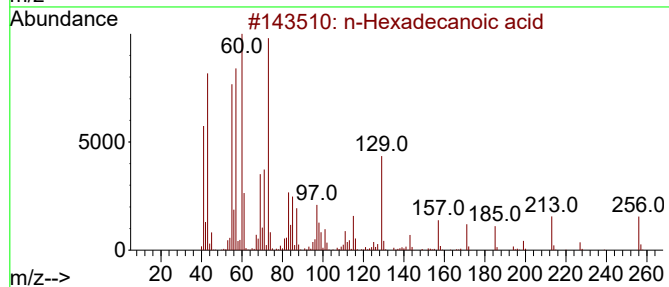
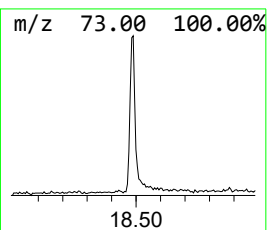
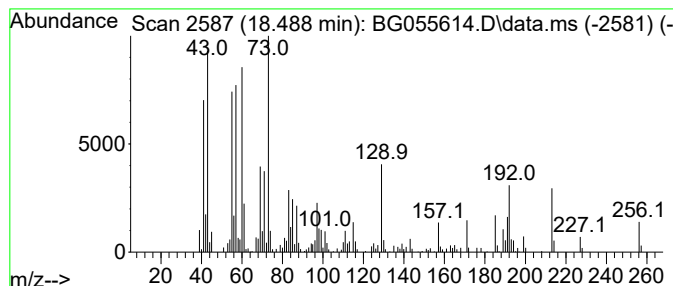
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	6.79 ng	265778	Phenanthrene-d10	17.624

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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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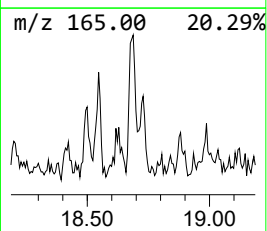
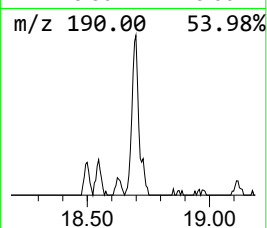
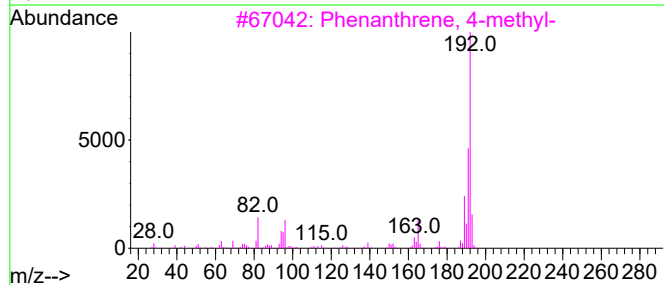
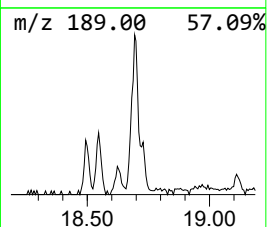
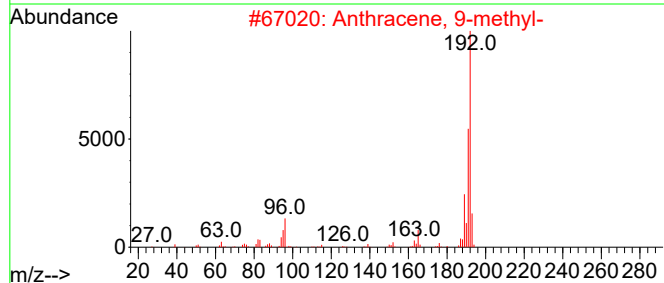
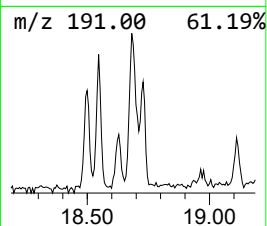
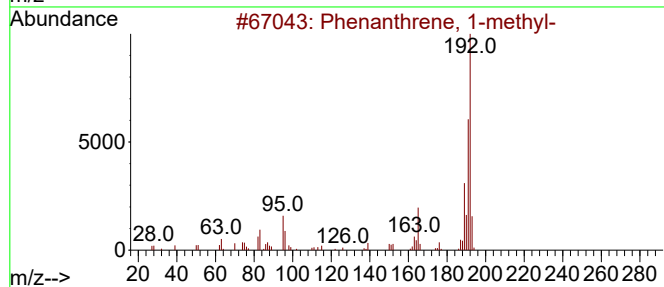
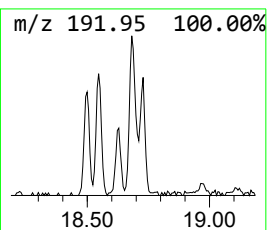
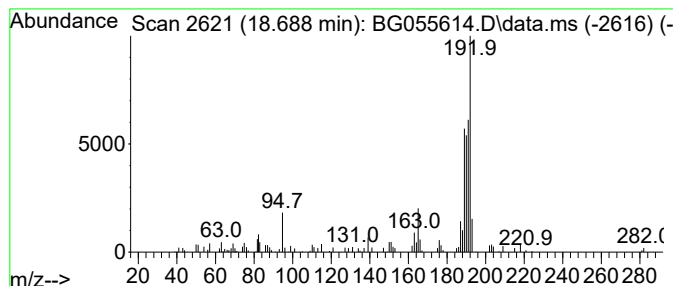
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Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.688	2.50 ng	97847	Phenanthrene-d10	17.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	83
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	64
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	64
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	60
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55



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ClientSampleId :
SB-28A

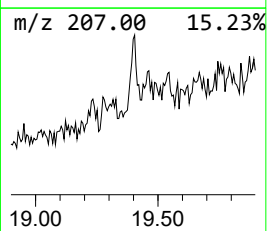
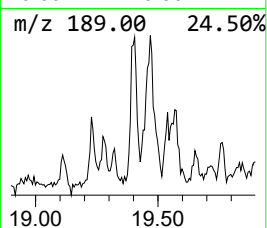
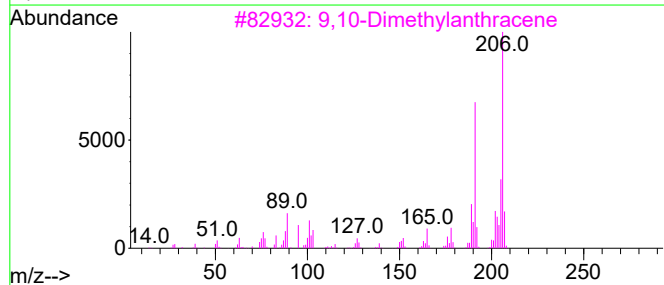
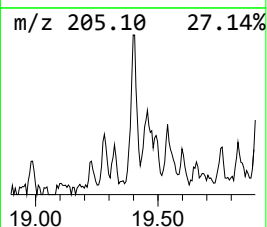
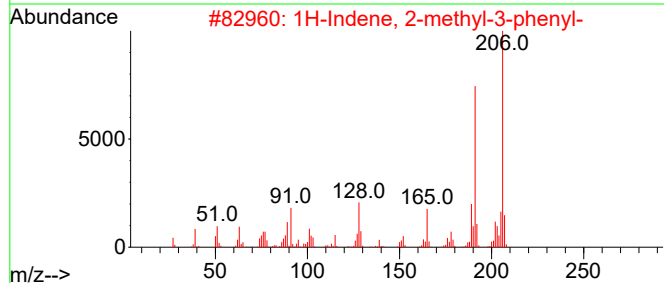
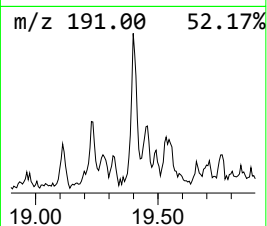
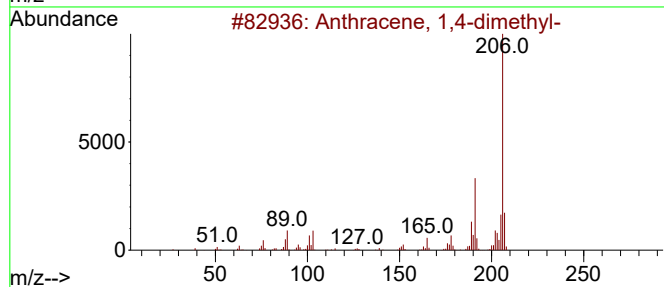
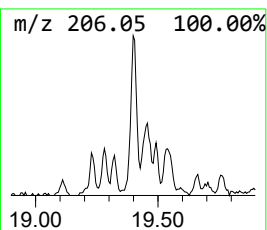
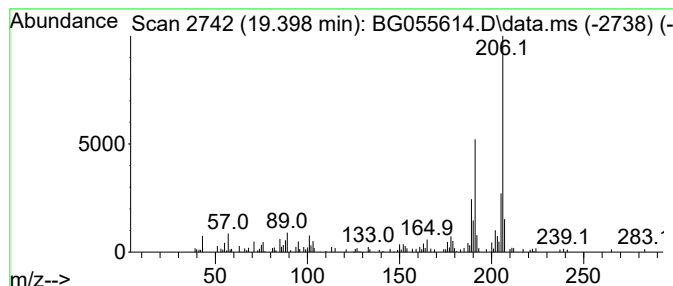
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Anthracene, 1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	3.24 ng	126856	Phenanthrene-d10	17.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
2			1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	93
3			9,10-Dimethylantracene	206	C16H14	000781-43-1	93
4			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
5			di-p-Tolylacetylene	206	C16H14	002789-88-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055614.D
Acq On : 14 Nov 2022 21:29
Operator : CG/JU
Sample : N5531-12
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28A

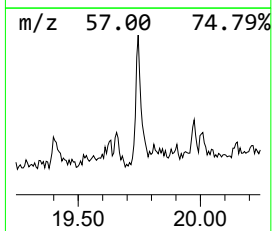
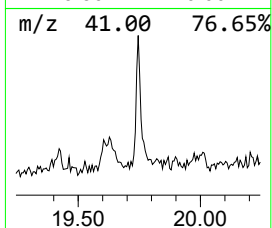
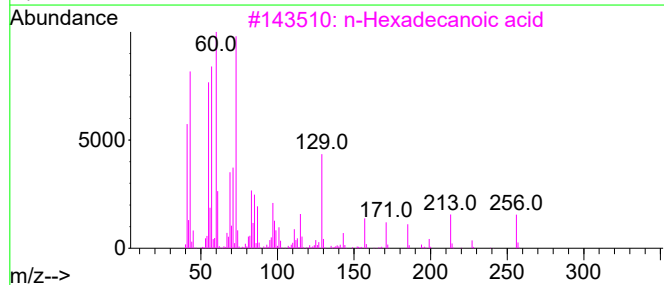
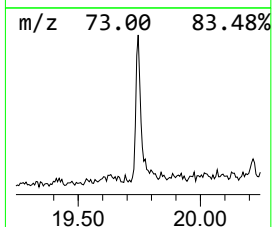
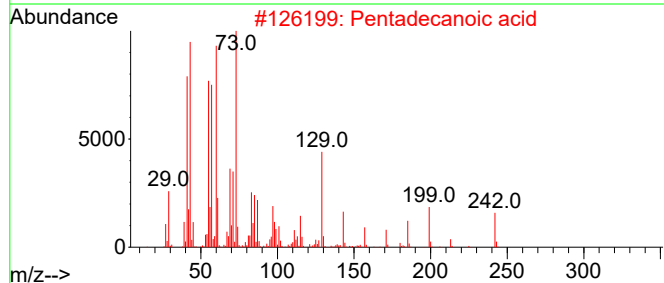
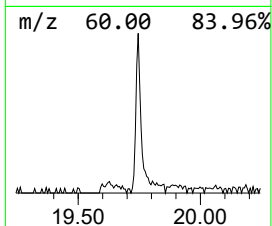
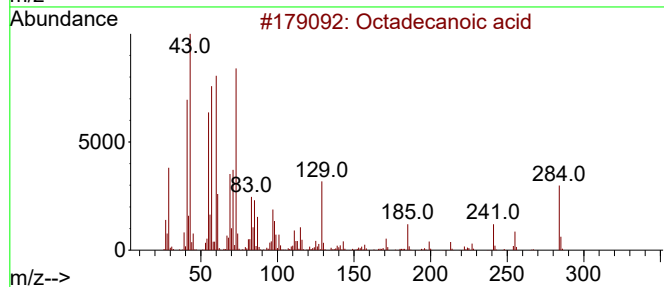
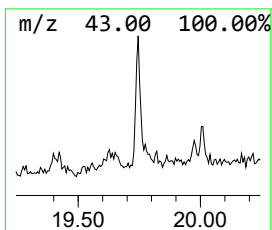
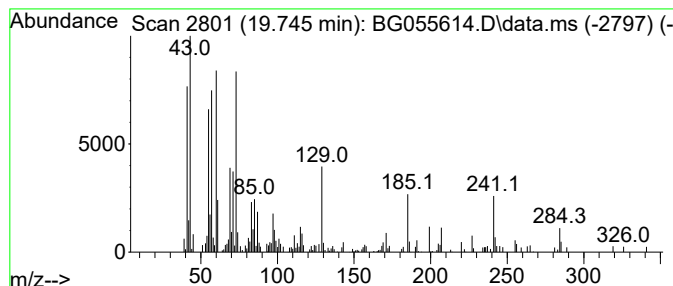
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.745	3.05 ng	119277	Phenanthrene-d10	17.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055614.D
Acq On : 14 Nov 2022 21:29
Operator : CG/JU
Sample : N5531-12
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28A

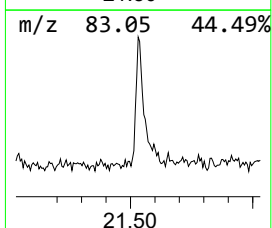
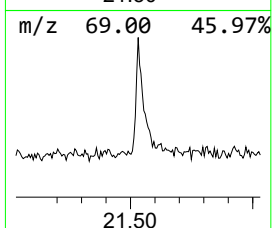
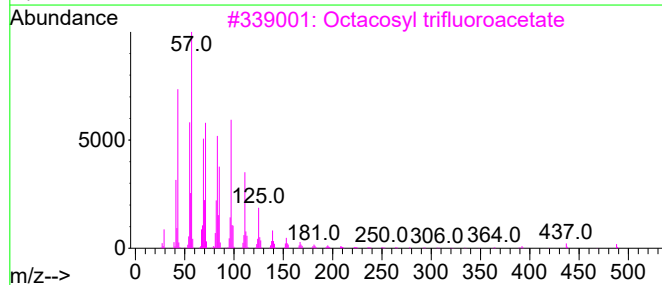
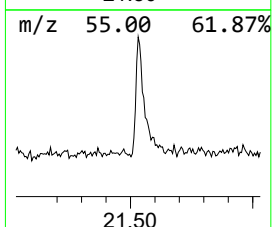
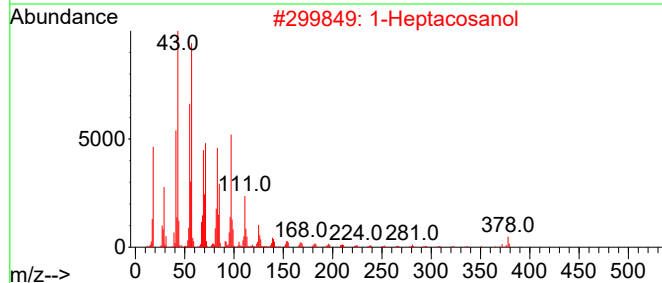
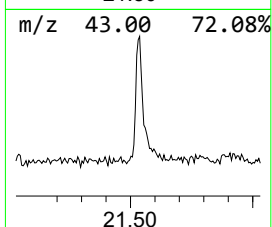
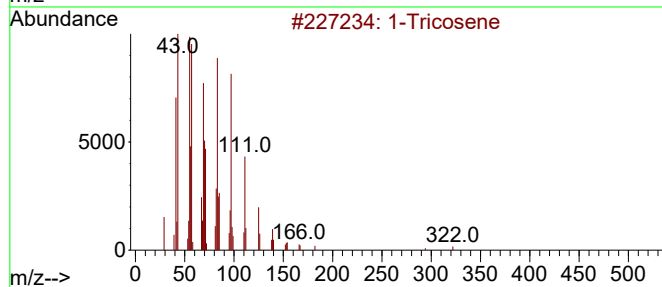
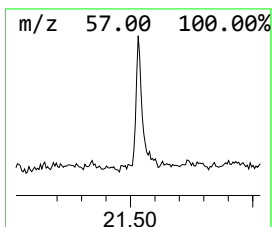
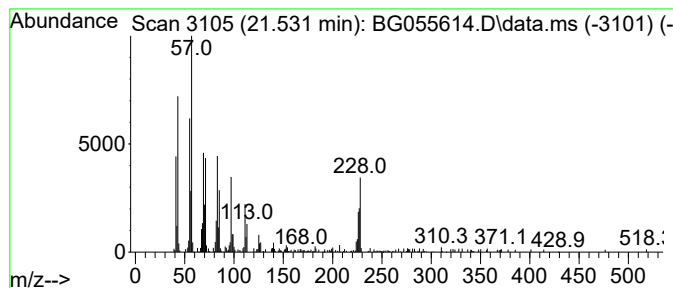
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.531	5.27 ng	241910	Chrysene-d12	21.931

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	87
2	1-Heptacosanol			396	C27H56O	002004-39-9	68
3	Octacosyl trifluoroacetate			506	C30H57F3O2	1000351-74-9	68
4	17-Pentatriacontene			491	C35H70	006971-40-0	68
5	Oxalic acid, isobutyl hexadecyl ...			370	C22H42O4	1000309-38-1	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055614.D
Acq On : 14 Nov 2022 21:29
Operator : CG/JU
Sample : N5531-12
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
Butane, 2-metho...	3.323	22.2	ng	356942	1	8.264	321283	20.0
2-Pentanone, 4-...	5.315	11.1	ng	178971	1	8.264	321283	20.0
Ethanol, 2-(2-b...	10.838	3.7	ng	89184	2	11.091	481428	20.0
n-Hexadecanoic ...	18.488	6.8	ng	265778	4	17.624	782996	20.0
Phenanthrene, 1...	18.688	2.5	ng	97847	4	17.624	782996	20.0
Anthracene, 1,4...	19.398	3.2	ng	126856	4	17.624	782996	20.0
Octadecanoic acid	19.745	3.0	ng	119277	4	17.624	782996	20.0
1-Tricosene	21.531	5.3	ng	241910	5	21.931	917289	20.0