

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121923\
 Data File : BG060096.D
 Acq On : 19 Dec 2023 22:11
 Operator : MA/JU
 Sample : 05759-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 AU-06-121323

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060096.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.141	3	9	19	rVB	87706	164032	3.75%	0.578%
2	5.063	331	336	342	rBV	28724	50091	1.14%	0.176%
3	5.527	407	415	424	rBV	722608	1173724	26.82%	4.133%
4	7.113	676	685	692	rBV	844780	1427177	32.61%	5.025%
5	7.953	821	828	834	rBV	260059	430795	9.84%	1.517%
6	9.111	1017	1025	1034	rBV	523671	888691	20.30%	3.129%
7	10.756	1296	1305	1312	rBV	330270	593776	13.57%	2.091%
8	13.212	1716	1723	1730	rVB	1817796	2615827	59.76%	9.211%
9	14.587	1949	1957	1965	rVB	597684	942664	21.54%	3.319%
10	15.433	2097	2101	2106	rVB	47475	58989	1.35%	0.208%
11	16.079	2204	2211	2219	rVB	1442626	2192229	50.08%	7.719%
12	16.273	2239	2244	2246	rBV2	60888	91691	2.09%	0.323%
13	16.296	2246	2248	2251	rVB2	36401	45714	1.04%	0.161%
14	17.090	2379	2383	2388	rBV	66924	91706	2.10%	0.323%
15	17.142	2389	2392	2403	rVB8	33714	65583	1.50%	0.231%
16	17.336	2418	2425	2431	rBV	844252	1231848	28.14%	4.337%
17	17.830	2506	2509	2513	rBV	63373	78602	1.80%	0.277%
18	18.006	2534	2539	2544	rVB	722913	860939	19.67%	3.031%
19	18.224	2571	2576	2581	rBV3	127890	201975	4.61%	0.711%
20	18.529	2622	2628	2631	rBV3	59960	77598	1.77%	0.273%
21	19.152	2728	2734	2737	rBV	3591128	4377047	100.00%	15.412%
22	19.181	2737	2739	2750	rVB2	2000787	2397426	54.77%	8.442%
23	19.311	2757	2761	2766	rVB	352260	416882	9.52%	1.468%
24	19.393	2771	2775	2781	rVV	115250	174749	3.99%	0.615%
25	19.452	2781	2785	2789	rVV4	48029	58832	1.34%	0.207%
26	19.734	2829	2833	2834	rBV3	66226	77227	1.76%	0.272%
27	19.757	2834	2837	2845	rVB2	107565	184859	4.22%	0.651%
28	19.963	2866	2872	2877	rBV	3218677	4160232	95.05%	14.649%
29	20.762	3006	3008	3012	rVB4	45303	50670	1.16%	0.178%
30	21.261	3089	3093	3099	rVB3	104515	161754	3.70%	0.570%
31	21.608	3146	3152	3158	rBV	931793	1516125	34.64%	5.338%
32	24.798	3687	3695	3709	rVB	533891	1540709	35.20%	5.425%

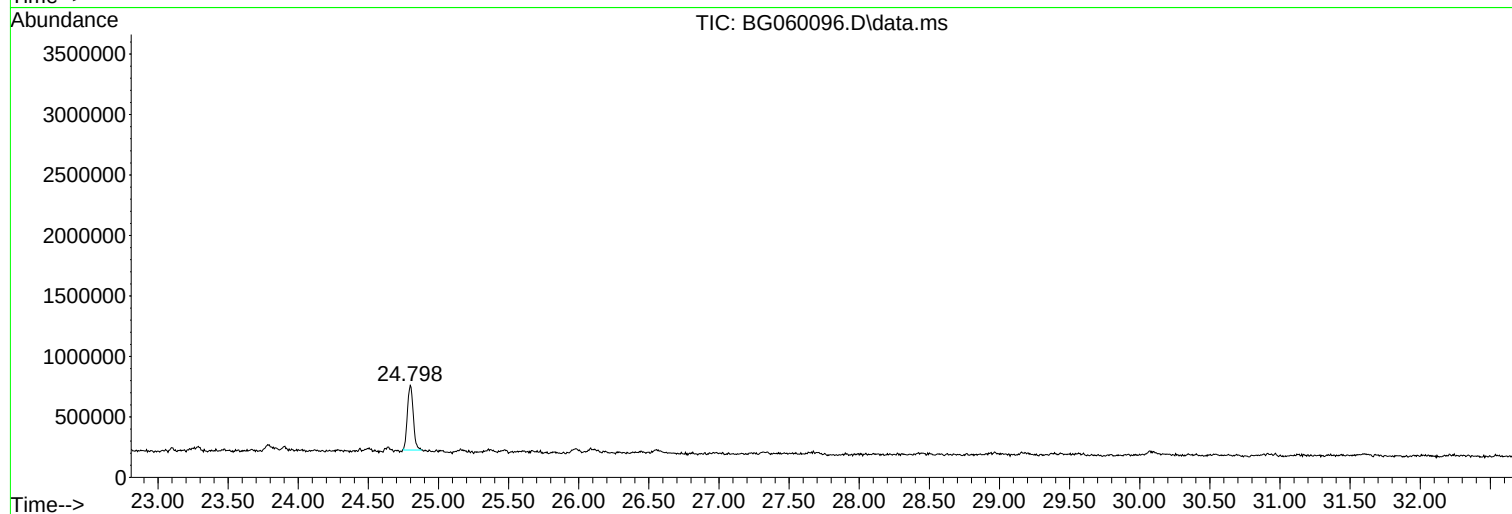
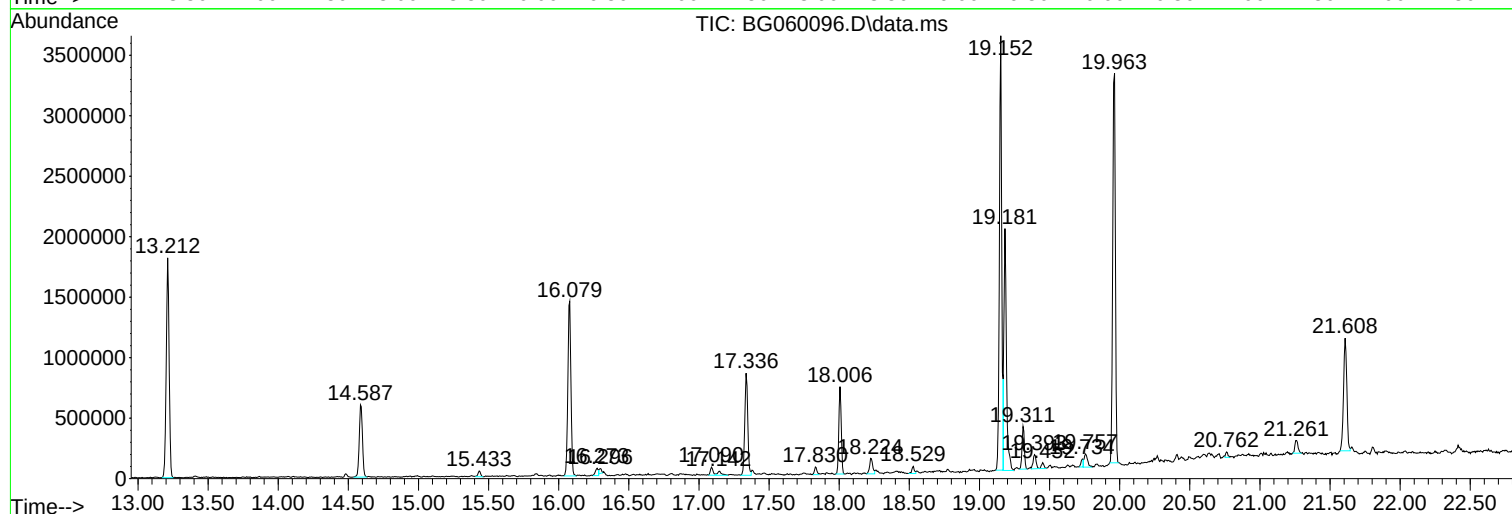
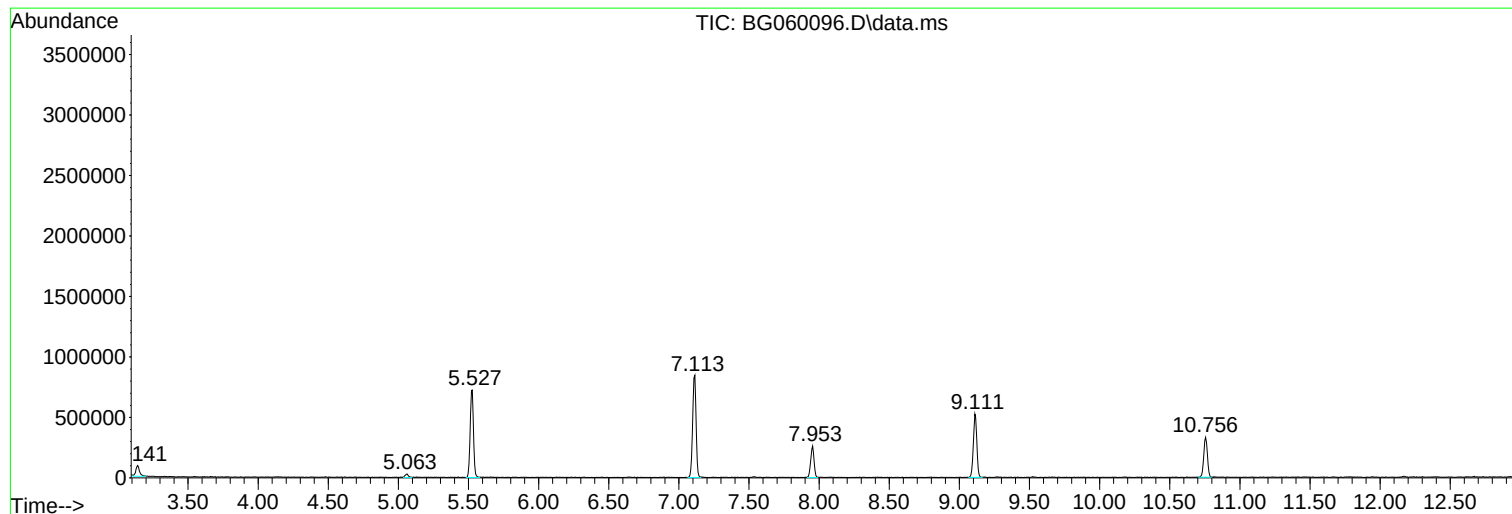
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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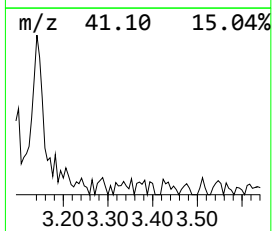
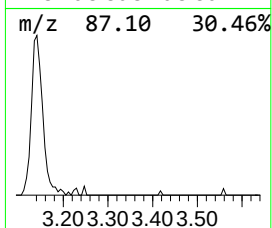
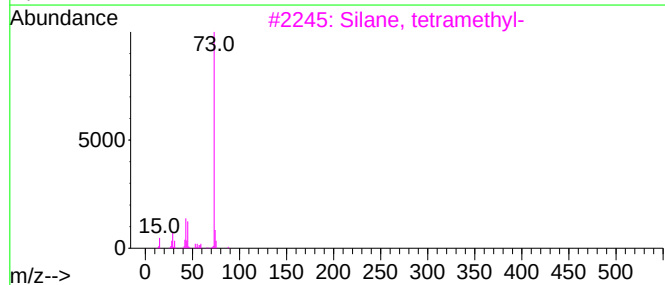
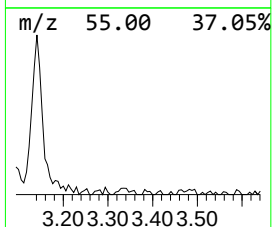
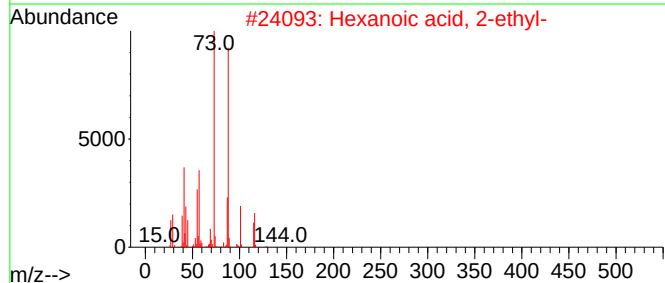
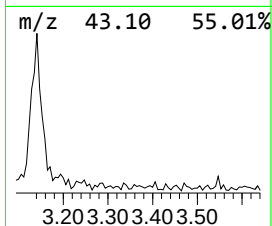
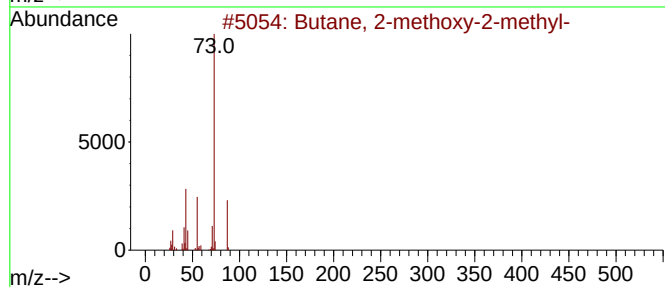
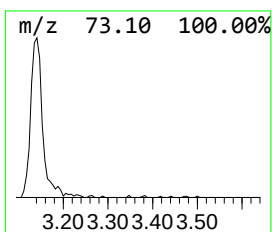
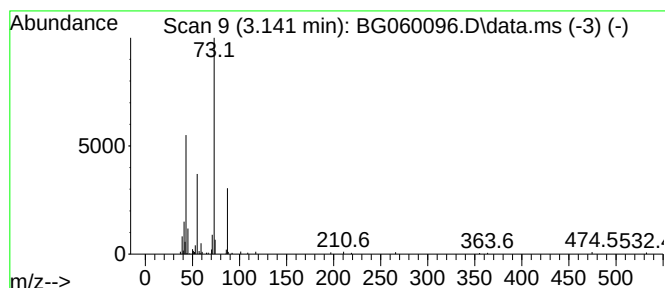
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.141 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.141	7.62 ng	164032	1,4-Dichlorobenzene-d4	7.953

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	40
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	36
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			8-Chloro-3,6-dioxaoctyl acetate	210	C8H15ClO4	1000322-41-5	23
5			Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	23



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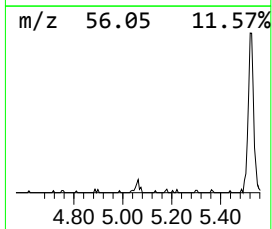
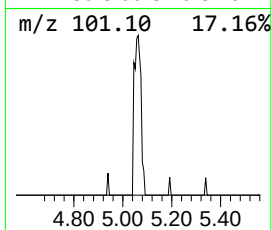
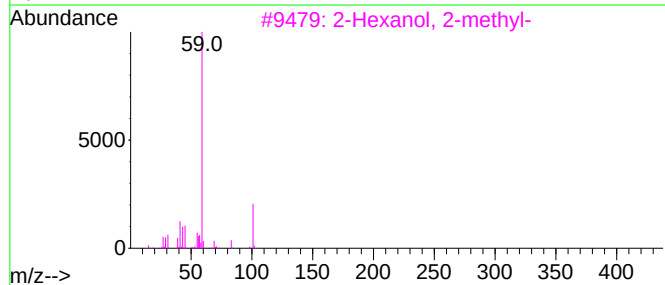
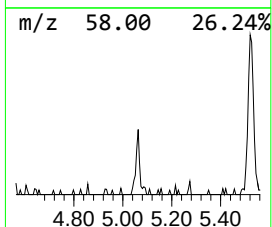
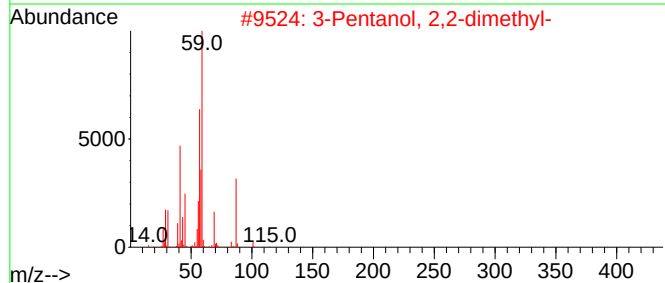
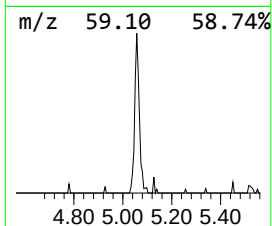
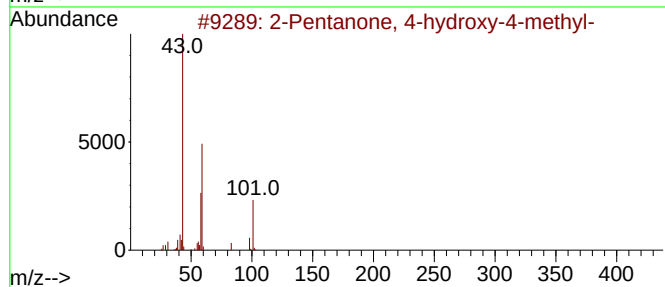
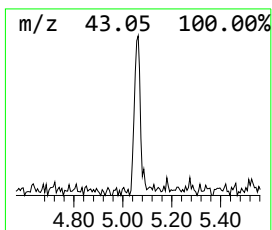
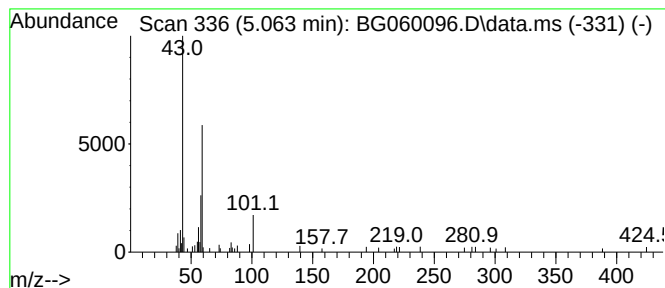
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	2.33 ng	50091	1,4-Dichlorobenzene-d4	7.953

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4			2-hydroxy-2-methyl-4-heptanone	144	C8H16O2	054862-91-8	36
5			Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	33



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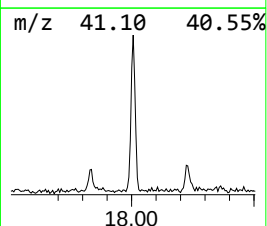
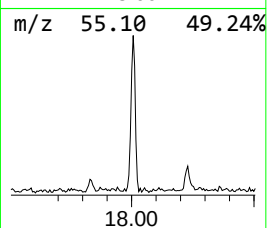
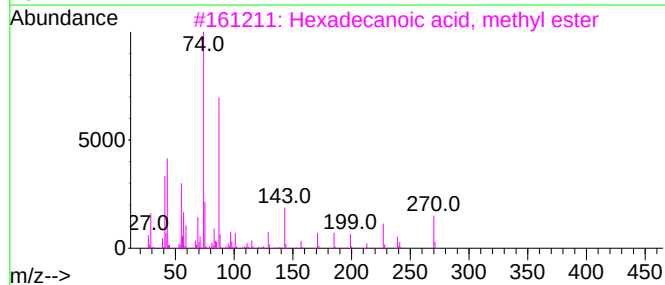
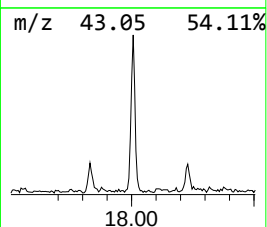
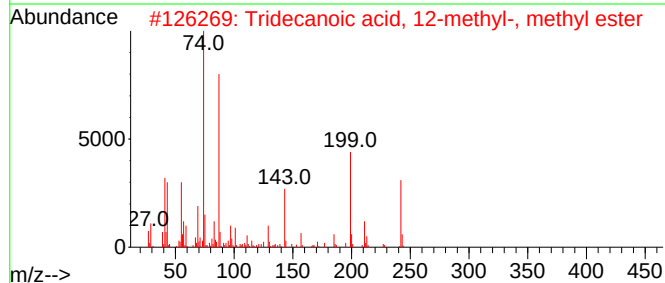
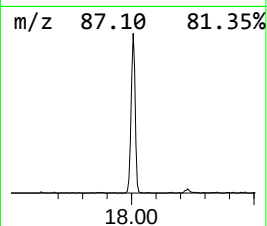
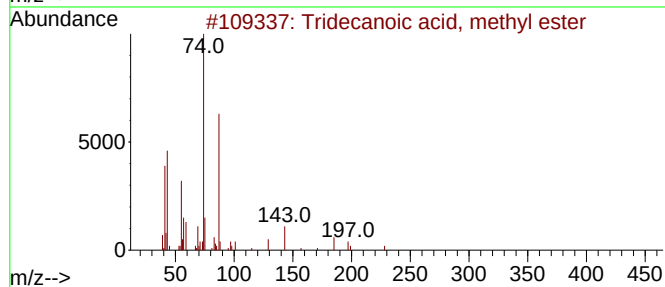
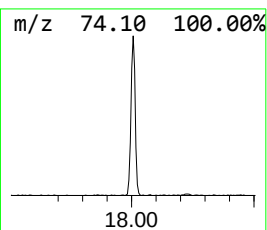
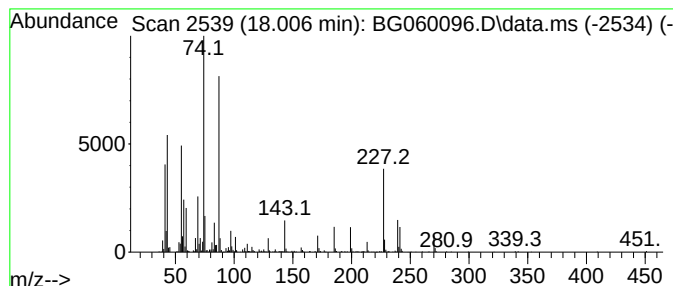
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tridecanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.006	13.98 ng	860939	Phenanthrene-d10	17.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
2			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	70
3			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	64
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	64
5			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	64



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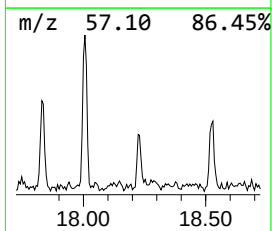
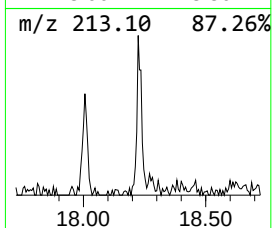
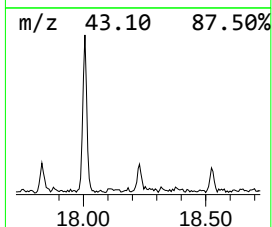
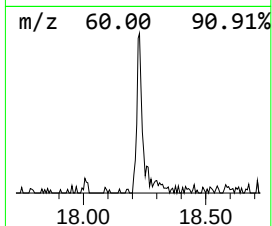
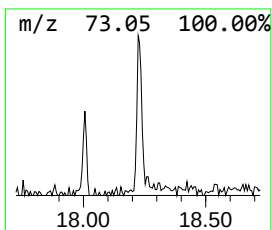
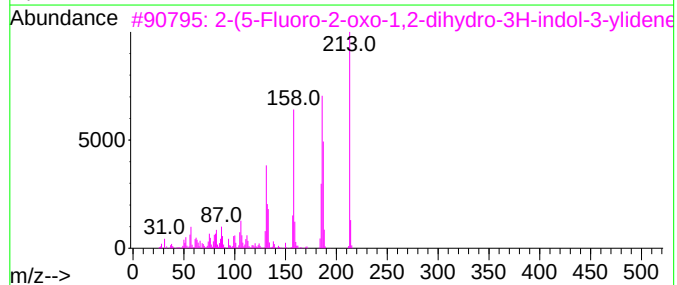
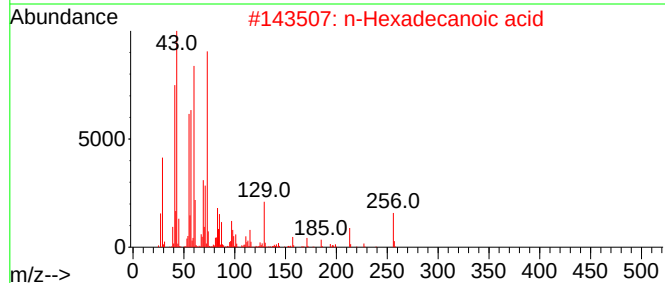
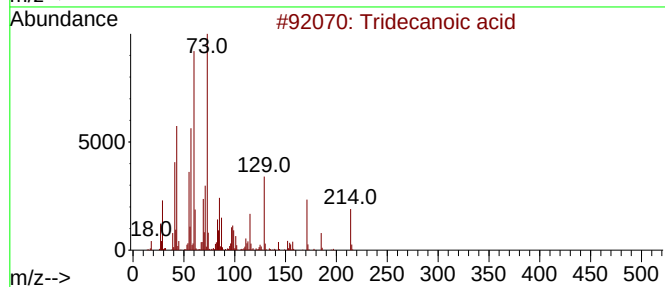
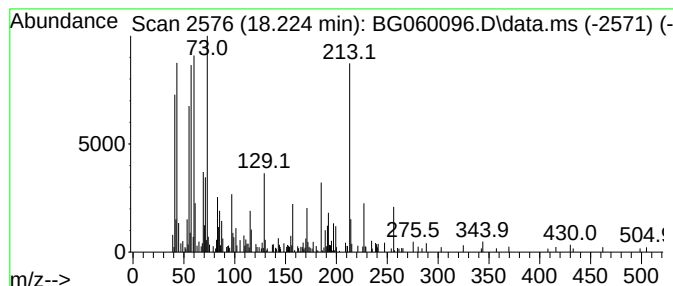
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Peak Number 4 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.224	3.28 ng	201975	Phenanthrene-d10	17.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	66
3			2-(5-Fluoro-2-oxo-1,2-dihydro-3H...	213	C11H4FN3O	116719-42-7	27
4			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	25
5			naphth[2,1-d]oxazole, 5-methoxy-...	213	C13H11NO2	1010396-17-7	20



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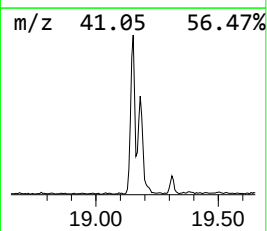
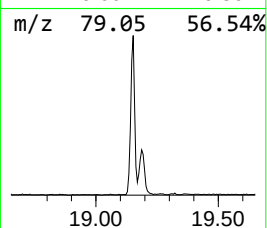
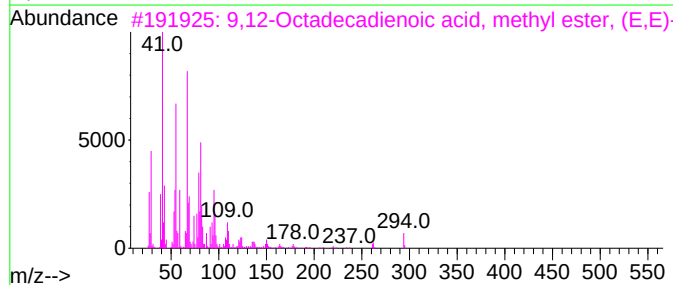
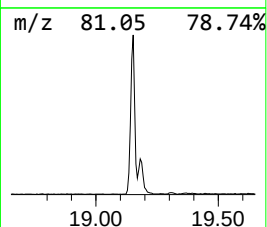
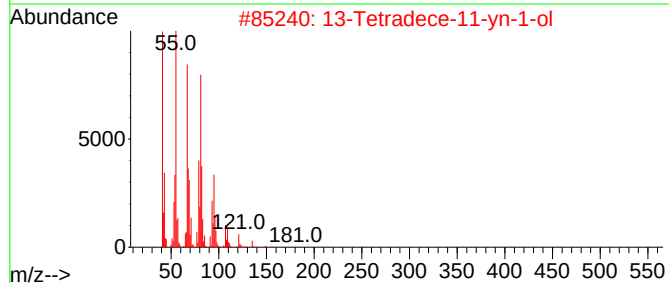
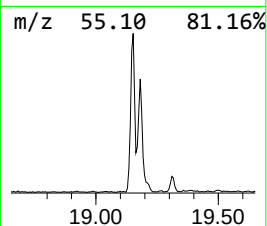
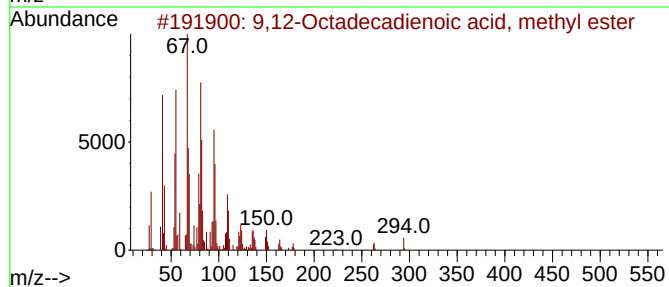
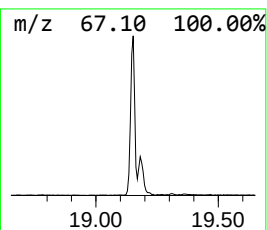
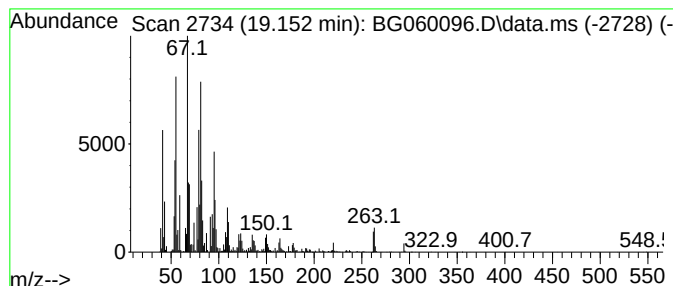
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Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.152	71.06 ng	4377050	Phenanthrene-d10	17.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	95
2			13-Tetradec-11-yn-1-ol	208	C14H24O	1000131-00-4	95
3			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	93
4			9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	89
5			9,12-Octadecadienal	264	C18H32O	026537-70-2	89



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ALS Vial : 16 Sample Multiplier: 1

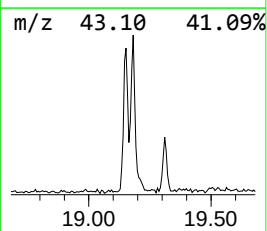
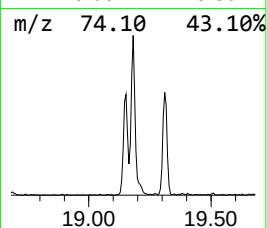
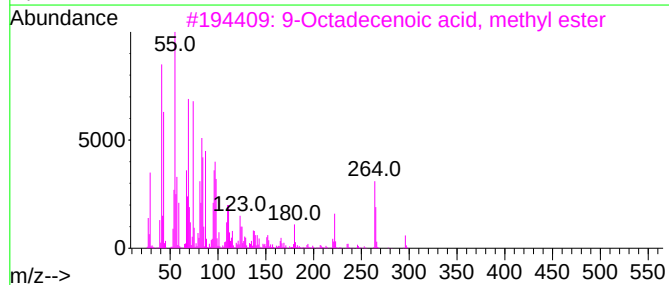
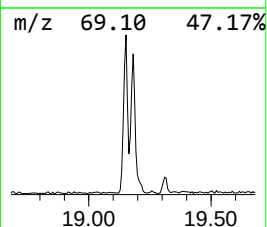
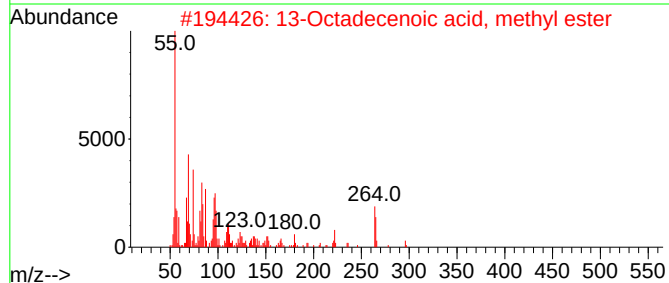
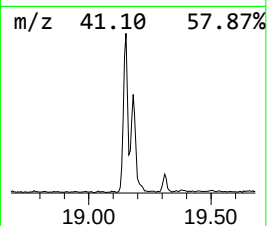
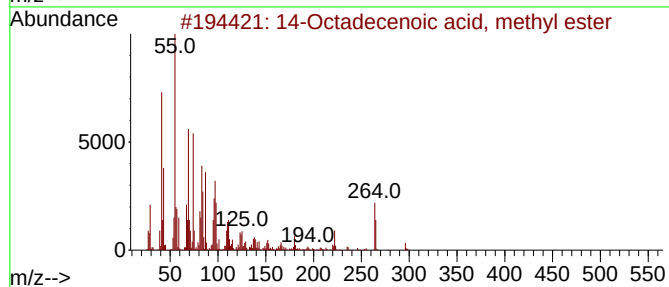
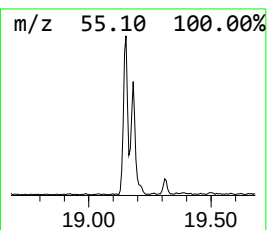
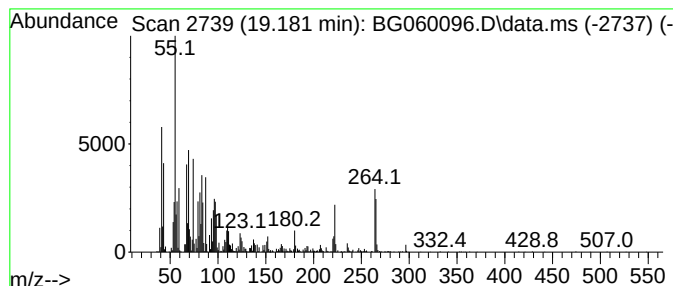
Instrument :
BNA_G
ClientSampleId :
AU-06-121323

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 14-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.181	38.92 ng	2397430	Phenanthrene-d10	17.336	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	96
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	96
3	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	96
4	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	95
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121923\
Data File : BG060096.D
Acq On : 19 Dec 2023 22:11
Operator : MA/JU
Sample : 05759-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-06-121323

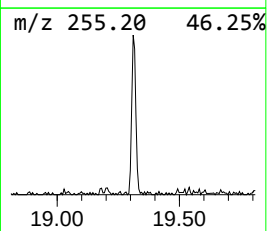
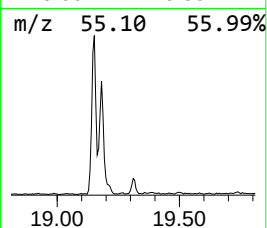
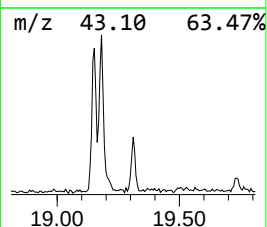
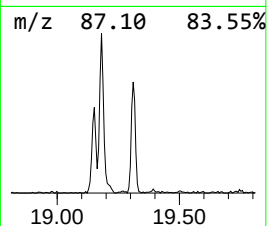
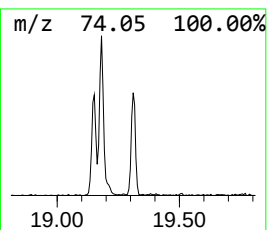
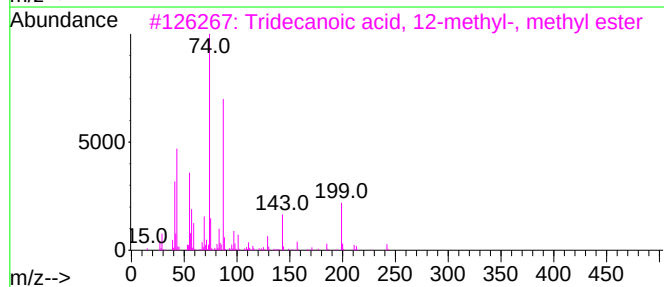
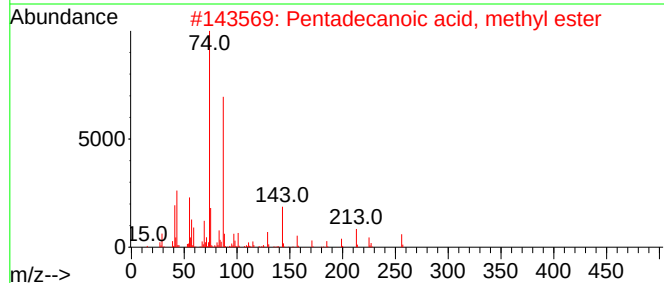
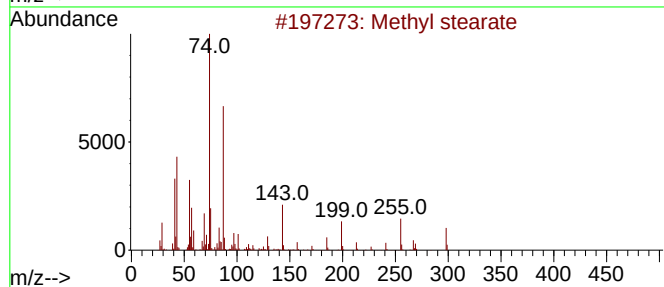
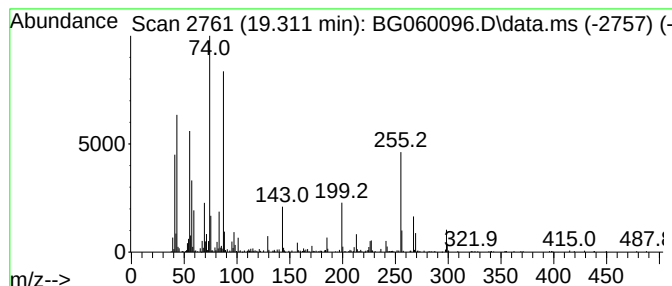
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.311	6.77 ng	416882	Phenanthrene-d10	17.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	93
2			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
3			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86
4			Tetradecanoic acid, 12-methyl-, ...	256	C16H32O2	005129-66-8	70
5			Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121923\
Data File : BG060096.D
Acq On : 19 Dec 2023 22:11
Operator : MA/JU
Sample : 05759-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-06-121323

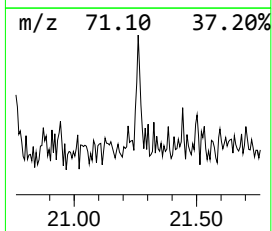
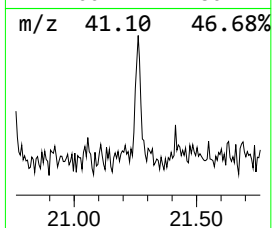
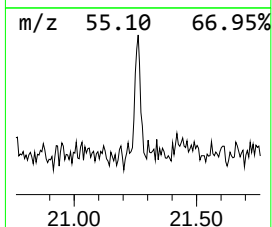
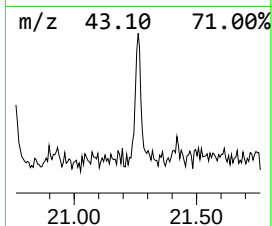
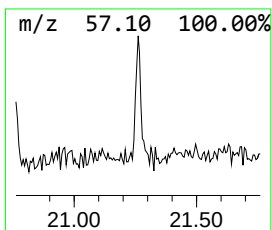
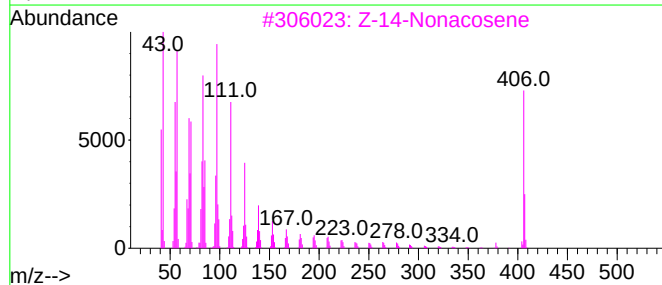
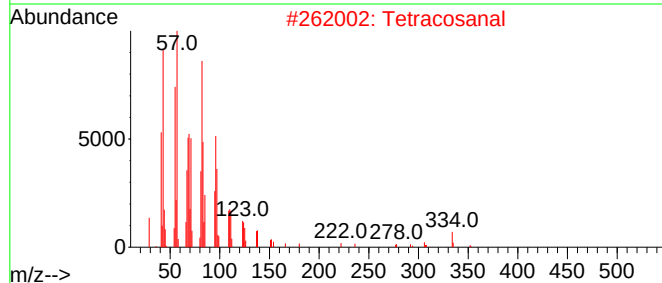
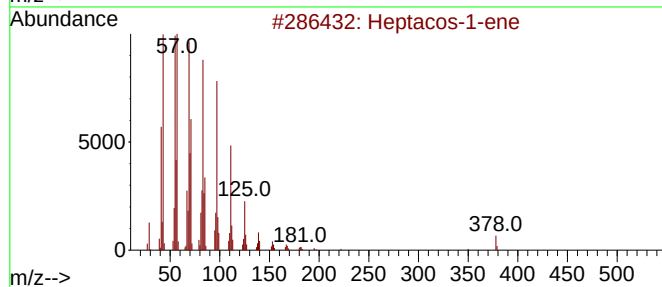
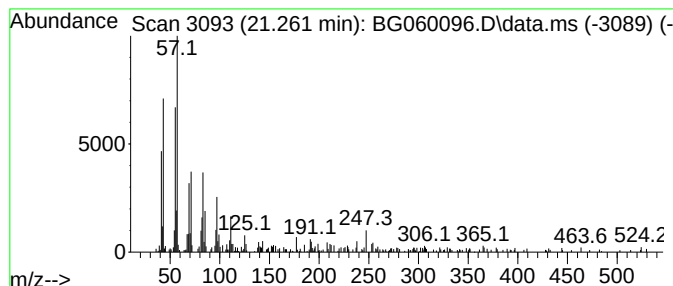
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacos-1-ene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.261	2.13 ng	161754	Chrysene-d12	21.608

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacos-1-ene	378	C27H54	015306-27-1	53
2			Tetracosanal	352	C24H48O	057866-08-7	42
3			Z-14-Nonacosene	406	C29H58	1010131-18-9	42
4			Hexacosyl propyl ether	424	C29H60O	1000406-28-4	38
5			Propyl triacontyl ether	481	C33H68O	1000406-28-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121923\
Data File : BG060096.D
Acq On : 19 Dec 2023 22:11
Operator : MA/JU
Sample : 05759-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-06-121323

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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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2-Pentanone, 4-...	5.063	2.3	ng	50091	1	7.953	430795	20.0
Tridecanoic aci...	18.006	14.0	ng	860939	4	17.336	1231850	20.0
Tridecanoic acid	18.224	3.3	ng	201975	4	17.336	1231850	20.0
9,12-Octadecadi...	19.152	71.1	ng	4377050	4	17.336	1231850	20.0
14-Octadecenoic...	19.181	38.9	ng	2397430	4	17.336	1231850	20.0
Methyl stearate	19.311	6.8	ng	416882	4	17.336	1231850	20.0
Heptacos-1-ene	21.261	2.1	ng	161754	5	21.608	1516130	20.0