LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060033.D
Acq On : 15 Dec 2023 13:08
Operator : MA/JU
Sample : 05791-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-K-O

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: BG060033.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.143	4	9	20	rVB	560655	917094	8.67%	2.423%
2	3.560	74	80	95	rBV	7045534	10579061	100.00%	27.953%
3	5.523	408	414	421	rBV	427782	670181	6.33%	1.771%
4	5.599	423	427	436	rVB2	94471	172137	1.63%	0.455%
5	6.316	543	549	559	rVB2	274804	396715	3.75%	1.048%
6	7.109	677	684	691	rBV	284904	456303	4.31%	1.206%
7	7.955	821	828	834	rBV	204820	338969	3.20%	0.896%
8	9.118	1019	1026	1038	rVB	620931	1131996	10.70%	2.991%
9	10.763	1295	1306	1311	rBV	265881	506920	4.79%	1.339%
10	13.214	1717	1723	1733	rVB	2130416	3317821	31.36%	8.767%
11	14.594	1952	1958	1965	rVB	502698	825551	7.80%	2.181%
12	15.029	2028	2032	2041	rVB2	165523	232167	2.19%	0.613%
13	16.081	2204	2211	2216	rBV	2198108	3218206	30.42%	8.503%
14	17.338	2417	2425	2431	rBV	783589	1201954	11.36%	3.176%
15	17.626	2468	2474	2479	rBV	674377	830961	7.85%	2.196%
16	18.231	2571	2577	2588	rBV2	152467	245042	2.32%	0.647%
17	19.389	2767	2774	2784	rBV7	73573	139834	1.32%	0.369%
18	19.506	2790	2794	2801	rBV5	97529	136185	1.29%	0.360%
19	19.964	2865	2872	2878	rBV	6412576	8284092	78.31%	21.889%
20	21.610	3146	3152	3158	rBV	1105938	1751346	16.55%	4.628%
21	24.800	3685	3695	3706	rBV	640069	1813454	17.14%	4.792%
22	29.430	4473	4483	4491	rBV5	152235	679926	6.43%	1.797%

Sum of corrected areas: 37845915

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
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Misc :
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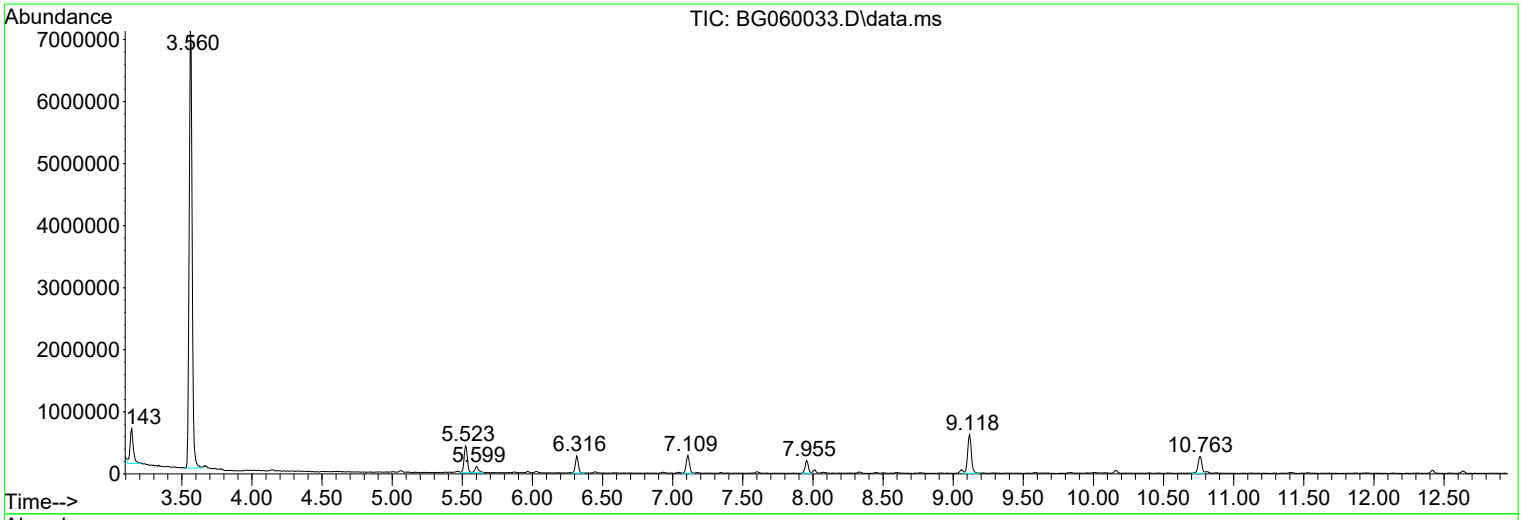
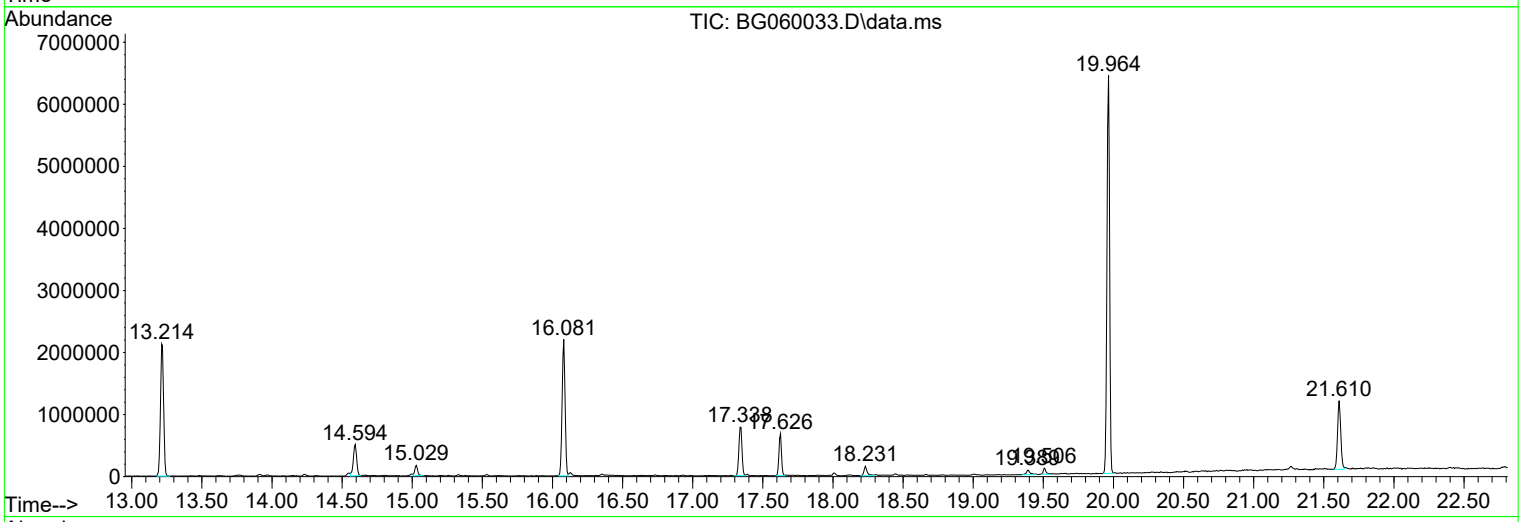
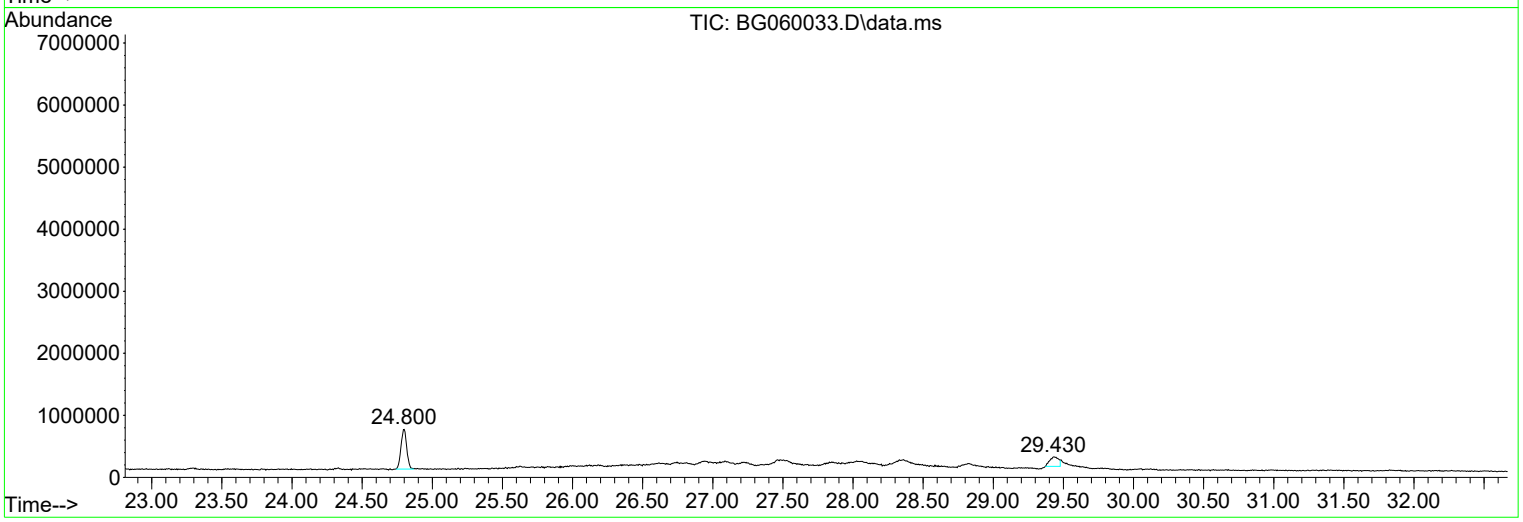
Instrument :
BNA_G
ClientSampleId :
597-K-O

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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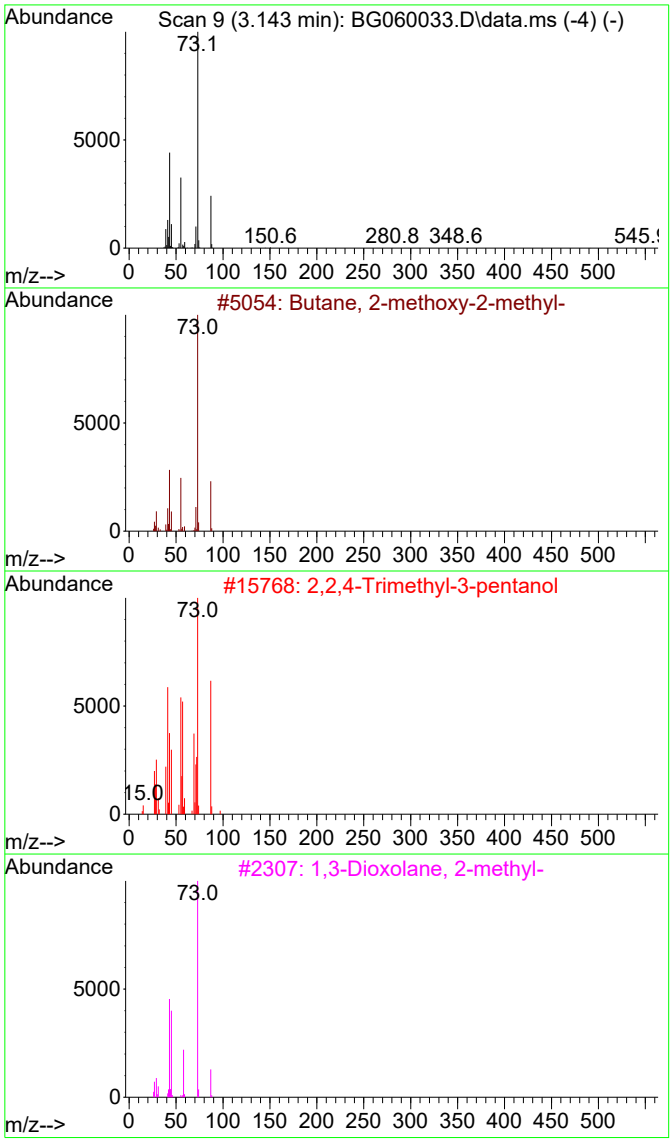
TIC Integration Parameters: LSCINT.P

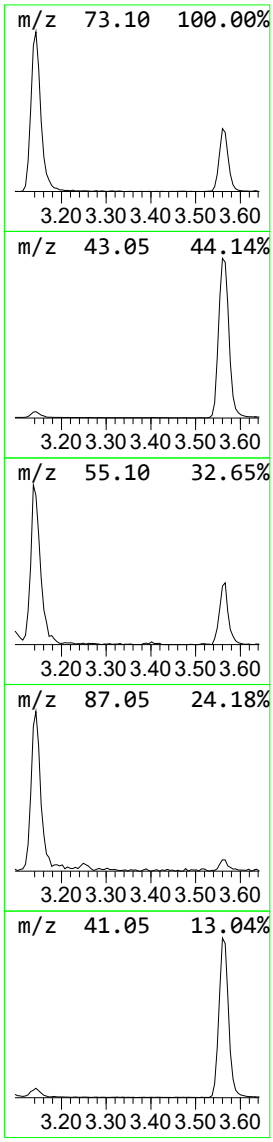
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	54.11 ng	917094	1,4-Dichlorobenzene-d4	7.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	28





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Data File : BG060033.D
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Operator : MA/JU
Sample : 05791-02
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Instrument :
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ClientSampleId :
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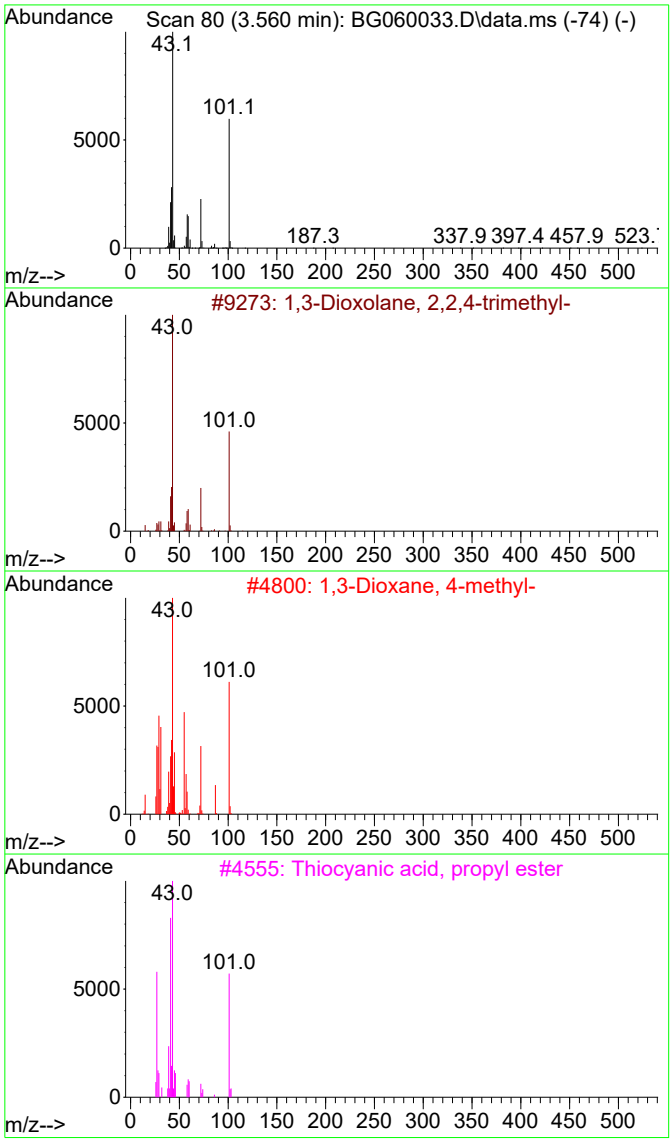
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

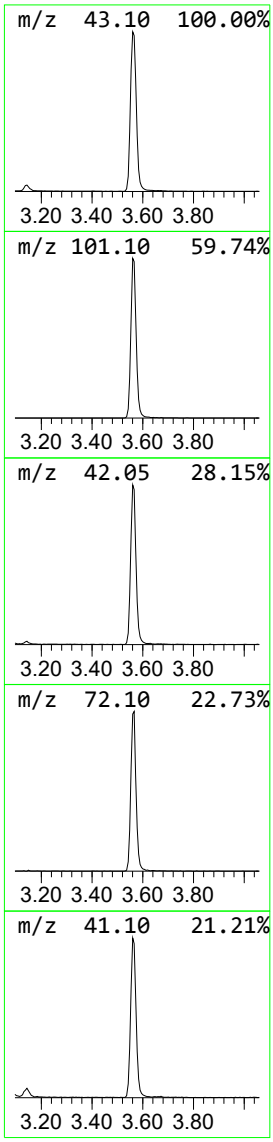
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.560	624.19 ng	10579100	1,4-Dichlorobenzene-d4	7.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	56
3	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	53
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	50
5	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	33





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Operator : MA/JU
Sample : 05791-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-K-O

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
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TIC Library : C:\Database\NIST20.L
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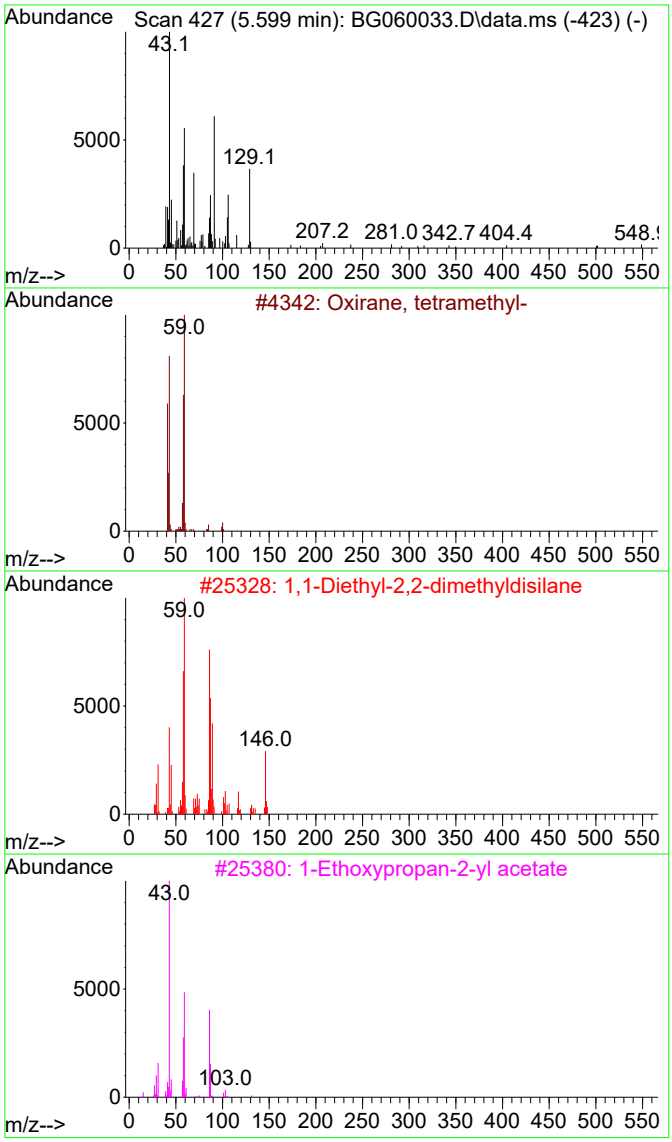
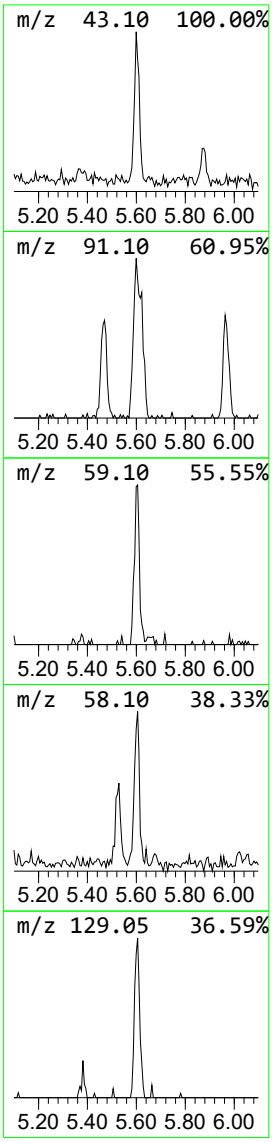
****

Peak Number 3 unknown5.599 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.599	10.16 ng	172137	1,4-Dichlorobenzene-d4	7.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	38
2	1,1-Diethyl-2,2-dimethyldisilane	146	C6H18Si2	1000434-35-6	28
3	1-Ethoxypropan-2-yl acetate	146	C7H14O3	1000378-33-2	25
4	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	23
5	4-Heptadecanone	254	C17H34O	053685-77-1	12





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Acq On : 15 Dec 2023 13:08
Operator : MA/JU
Sample : 05791-02
Misc :
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Instrument :
BNA_G
ClientSampleId :
597-K-O

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

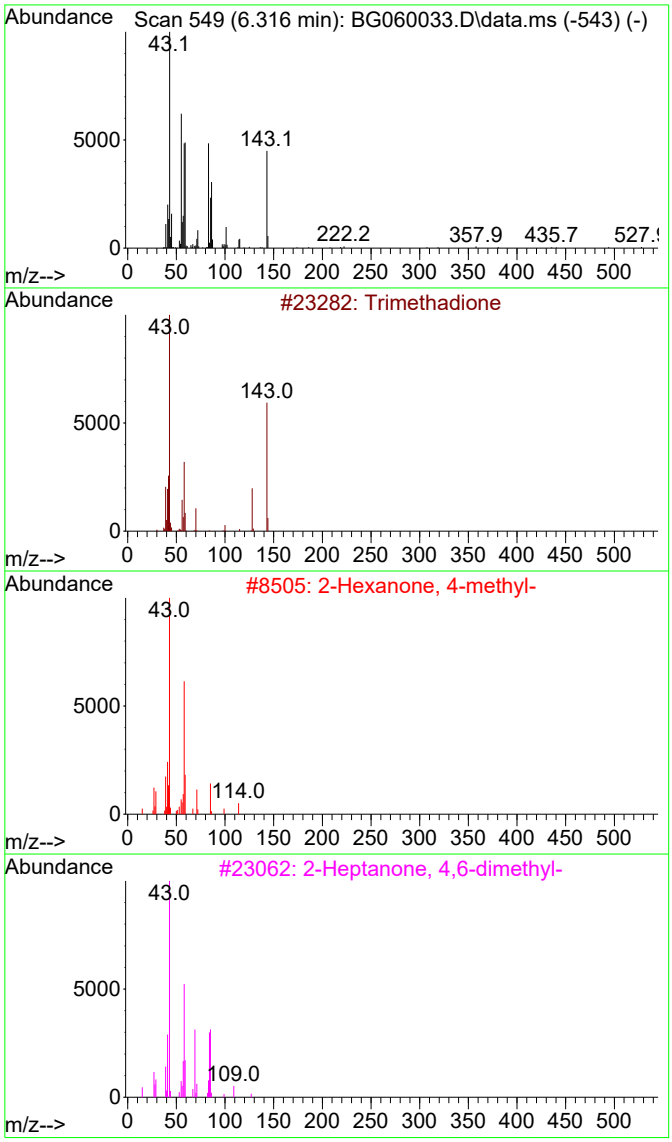
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

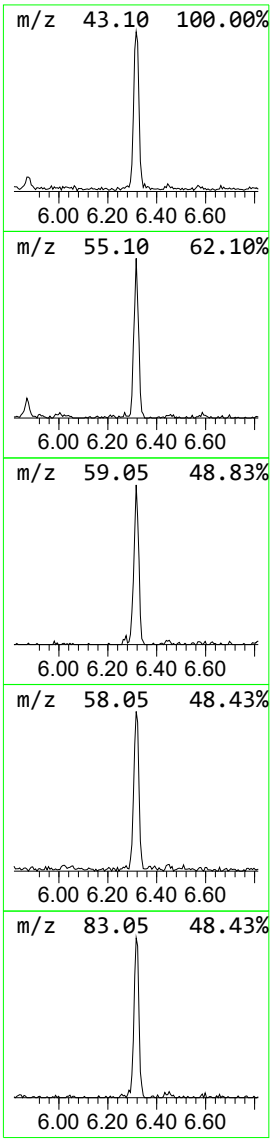
****

Peak Number 4 unknown6.316 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.316	23.41 ng	396715	1,4-Dichlorobenzene-d4	7.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethadione	143	C6H9NO3	000127-48-0	16
2	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	14
3	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	12
4	Terebic acid	158	C7H10O4	000079-91-4	12
5	1-(2,2-Dimethyl[1,3]dioxan-4-yl)...	160	C8H16O3	1000191-77-9	12





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Sample : 05791-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-K-O

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
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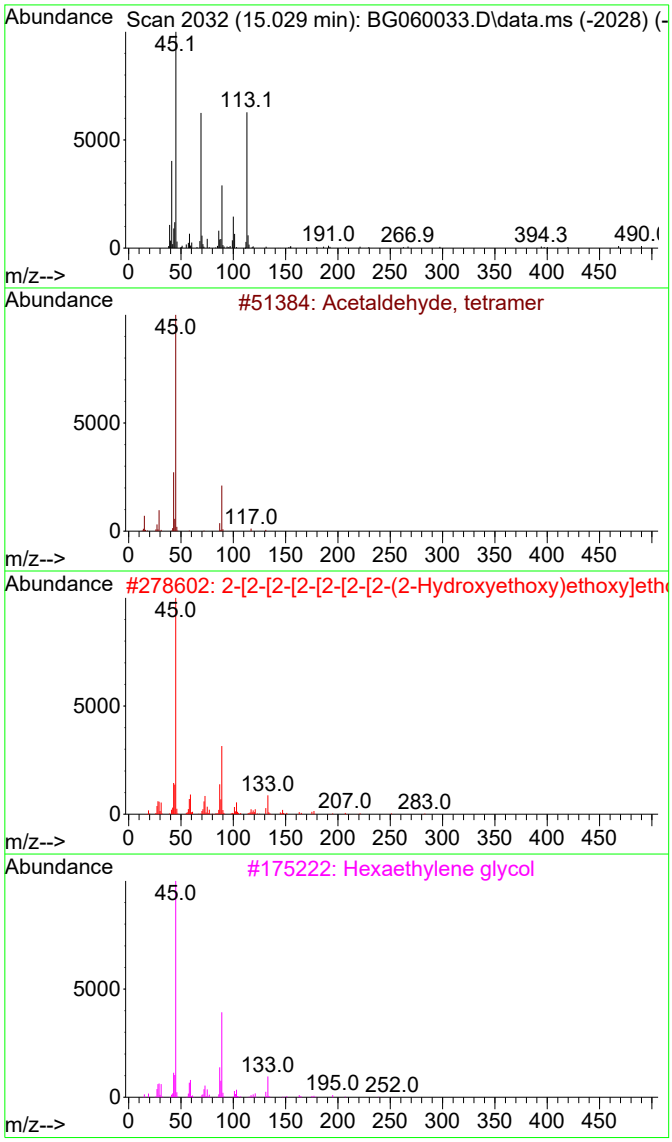
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

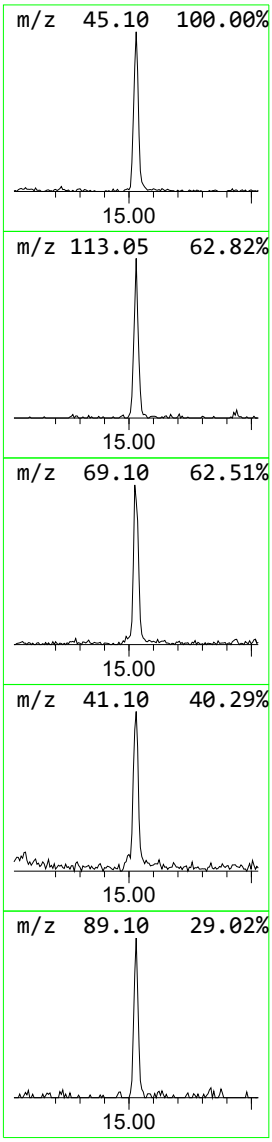
****

Peak Number 5 unknown15.029 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.029	5.62 ng	232167	Acenaphthene-d10	14.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	43
2	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	38
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	38
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	37
5	2-Octanol	130	C8H18O	000123-96-6	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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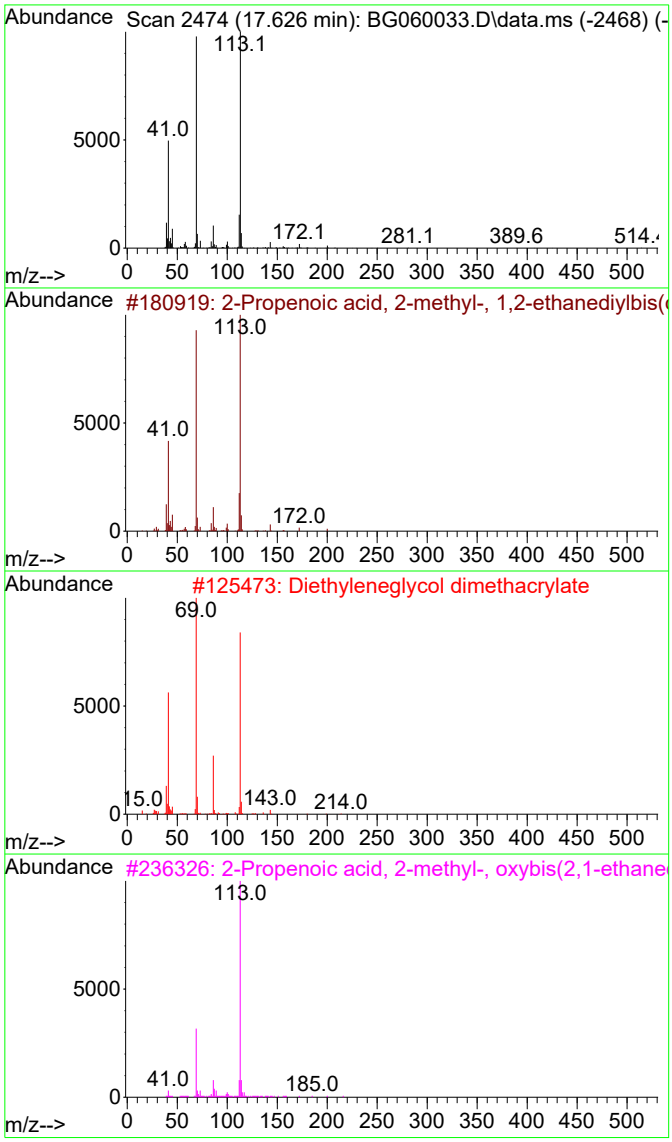
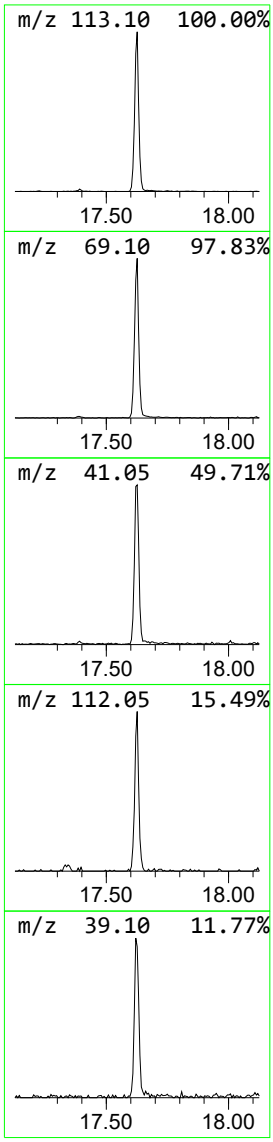
****
Peak Number 6 2-Propenoic acid, 2-methyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.626	13.83 ng	830961	Phenanthrene-d10	17.338

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-methyl-, 1,2...	286	C14H22O6	000109-16-0	91
2	Diethyleneglycol dimethacrylate	242	C12H18O5	002358-84-1	50
3	2-Propenoic acid, 2-methyl-, oxy...	330	C16H26O7	000109-17-1	43
4	3-Fluoro-5-hydroxypyridine	113	C5H4FNO	209328-55-2	38
5	2H-Pyrrol-2-one, 1,5-dihydro-4-m...	113	C5H7NO2	069778-83-2	32





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
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TIC Library : C:\Database\NIST20.L
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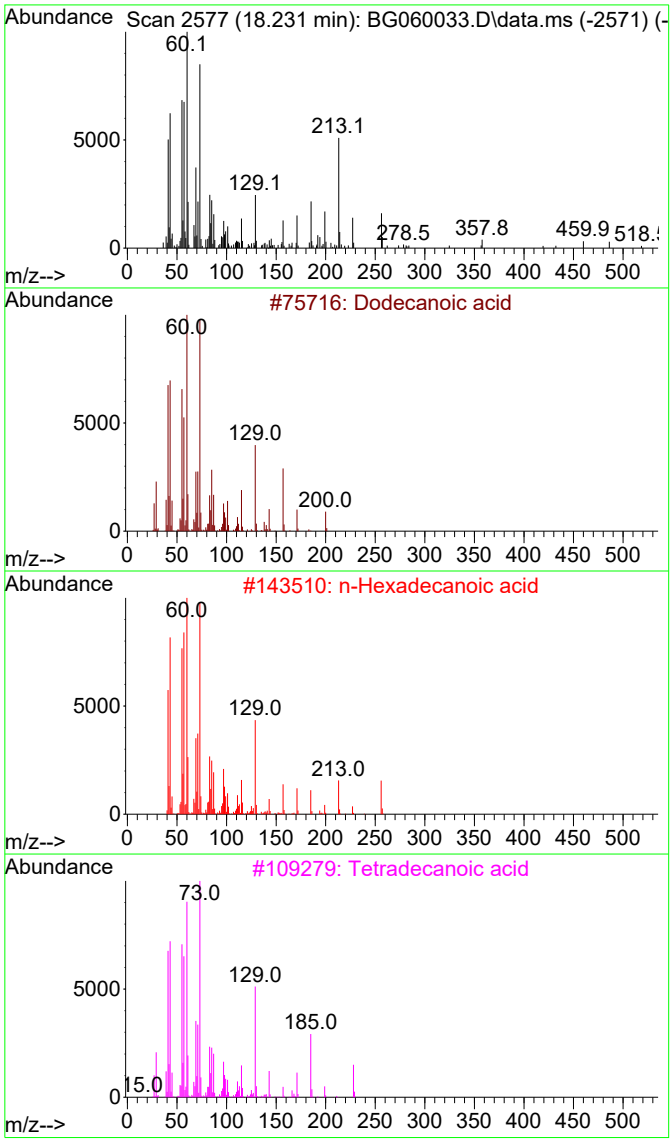
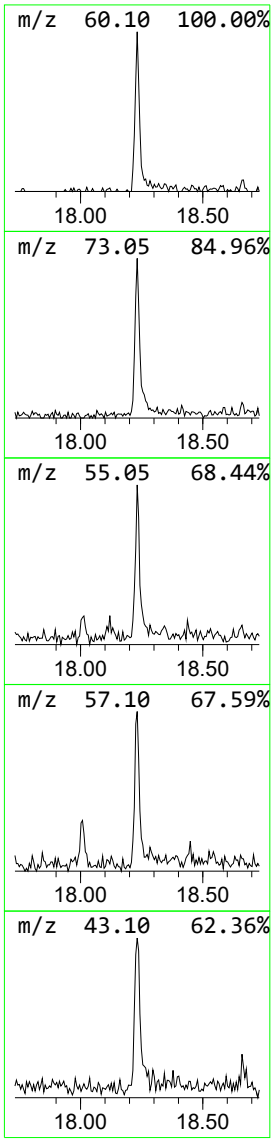
****

Peak Number 7 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.231	4.08 ng	245042	Phenanthrene-d10	17.338

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	92
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





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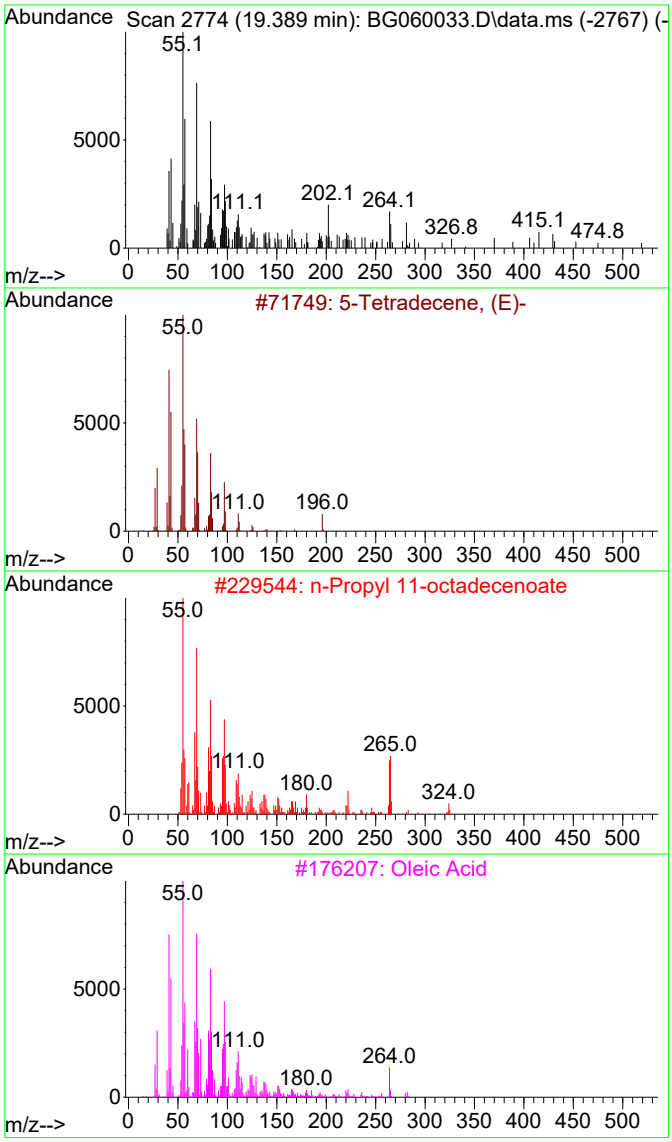
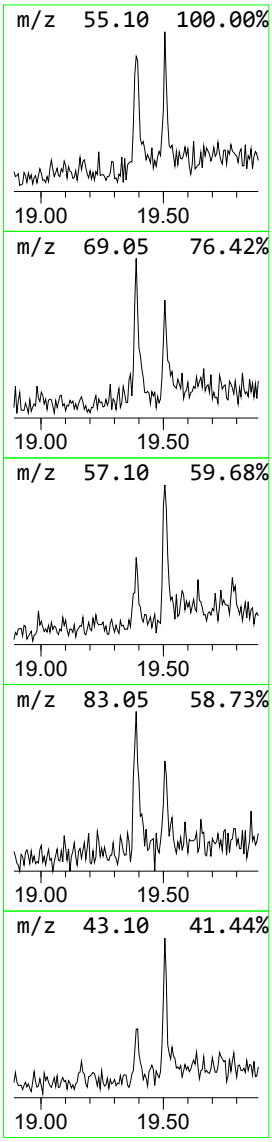
****

Peak Number 8 5-Tetradecene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.389	2.33 ng	139834	Phenanthrene-d10	17.338

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Tetradecene, (E)-	196	C14H28	041446-66-6	78
2	n-Propyl 11-octadecenoate	324	C21H40O2	1000336-71-7	58
3	Oleic Acid	282	C18H34O2	000112-80-1	55
4	6-Pentadecenoic acid, 13-methyl-...	254	C16H30O2	682751-34-4	53
5	3-Hexene, 2-methyl-, (E)-	98	C7H14	000692-24-0	49





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Instrument :
BNA_G
ClientSampleId :
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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
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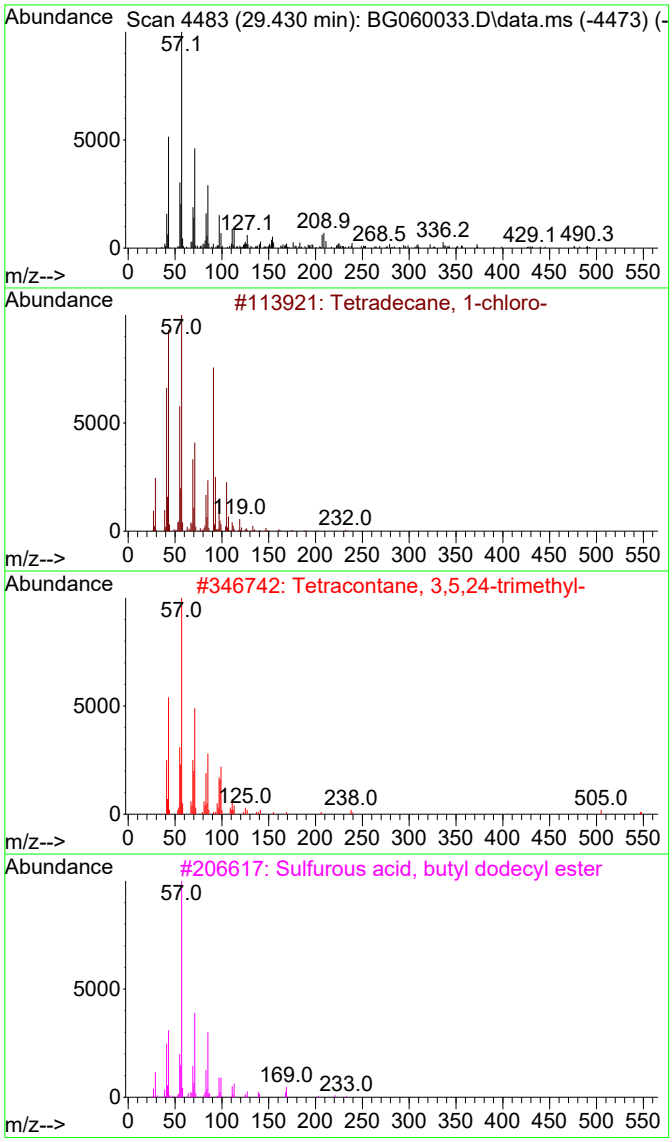
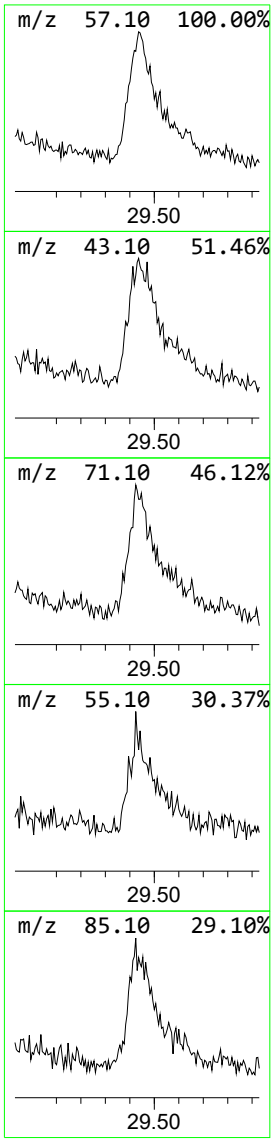
****

Peak Number 9 Tetradecane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.430	7.50 ng	679926	Perylene-d12	24.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	87
2	Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	86
3	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
4	Dotriacontane	451	C32H66	000544-85-4	86
5	Hexatriacontane	507	C36H74	000630-06-8	86





Tentatively Identified Compound (LSC) summary

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Data File : BG060033.D
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Sample : 05791-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-K-O

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.143	54.1	ng	917094	1	7.961	338969	20.0
1,3-Dioxolane, ...	3.560	624.2	ng	10579100	1	7.961	338969	20.0
unknown5.599	5.599	10.2	ng	172137	1	7.961	338969	20.0
unknown6.316	6.316	23.4	ng	396715	1	7.961	338969	20.0
unknown15.029	15.029	5.6	ng	232167	3	14.594	825551	20.0
2-Propenoic aci...	17.626	13.8	ng	830961	4	17.338	1201950	20.0
Dodecanoic acid	18.231	4.1	ng	245042	4	17.338	1201950	20.0
5-Tetradecene, ...	19.389	2.3	ng	139834	4	17.338	1201950	20.0
Tetradecane, 1-...	29.430	7.5	ng	679926	6	24.794	1813450	20.0