LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

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-BG032924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.099	15	19	27	rVV4	27464	50879	1.05%	0.168%
2	3.175	27	32	45	rVB	446137	624587	12.85%	2.067%
3	3.680	114	118	126	rBV	45686	64124	1.32%	0.212%
4	5.531	426	433	442	rBV	909604	1437137	29.57%	4.757%
5	7.112	692	702	711	rBV	1065258	1787137	36.78%	5.915%
6	7.952	837	845	853	rBV	236478	404704	8.33%	1.340%
7	9.103	1032	1041	1050	rBV	571984	1001259	20.60%	3.314%
8	10.531	1276	1284	1293	rBV	250576	403589	8.31%	1.336%
9	10.749	1314	1321	1332	rBV	379236	669201	13.77%	2.215%
10	13.210	1733	1740	1750	rVB	1798441	2791620	57.45%	9.240%
11	14.579	1966	1973	1980	rBV	690462	1073201	22.09%	3.552%
12	16.066	2219	2226	2234	rBV	1575060	2358370	48.53%	7.806%
13	16.977	2376	2381	2389	rVB2	38713	62790	1.29%	0.208%
14	17.329	2434	2441	2445	rBV	891542	1371522	28.22%	4.540%
15	17.370	2445	2448	2453	rVB	191041	263728	5.43%	0.873%
16	17.729	2501	2509	2513	rBV3	52227	97552	2.01%	0.323%
17	18.246	2592	2597	2605	rVB2	230110	355429	7.31%	1.176%
18	18.398	2616	2623	2627	rBV3	33652	64163	1.32%	0.212%
19	18.680	2667	2671	2673	rBV	51156	60585	1.25%	0.201%
20	18.733	2677	2680	2686	rVB	108432	161589	3.33%	0.535%
21	19.115	2740	2745	2752	rVB4	35331	62790	1.29%	0.208%
22	19.256	2764	2769	2773	rBV	45251	70956	1.46%	0.235%
23	19.380	2785	2790	2796	rBV	499880	718778	14.79%	2.379%
24	19.521	2809	2814	2818	rBV3	70590	101176	2.08%	0.335%
25	19.738	2842	2851	2858	rBV2	327267	612053	12.60%	2.026%
26	19.955	2879	2888	2900	rBV	3646574	4859326	100.00%	16.084%
27	20.073	2903	2908	2913	rBV5	36084	82564	1.70%	0.273%
28	20.202	2926	2930	2933	rBV5	33976	61605	1.27%	0.204%
29	20.396	2959	2963	2968	rVB3	42075	64357	1.32%	0.213%
30	20.796	3027	3031	3042	rVB6	46002	99991	2.06%	0.331%
31	20.990	3060	3064	3069	rVB	104294	155446	3.20%	0.515%
32	21.172	3088	3095	3100	rBV2	54433	131750	2.71%	0.436%
33	21.225	3100	3104	3107	rBV2	50392	70612	1.45%	0.234%
34	21.283	3107	3114	3119	rBV2	214973	429533	8.84%	1.422%
35	21.524	3151	3155	3158	rBV2	56906	79733	1.64%	0.264%
36	21.589	3158	3166	3171	rVV2	982824	1883556	38.76%	6.234%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
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Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

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-BG032924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.636	3171	3174	3183	rVB	230968	388188	7.99%	1.285%
38	21.806	3199	3203	3207	rBV2	87340	136831	2.82%	0.453%
39	22.382	3296	3301	3306	rVB3	66716	119629	2.46%	0.396%
40	22.453	3309	3313	3321	rBV3	87324	179526	3.69%	0.594%
41	22.805	3366	3373	3380	rBV2	349813	626822	12.90%	2.075%
42	23.481	3483	3488	3494	rBV3	100117	188583	3.88%	0.624%
43	23.733	3522	3531	3539	rBV2	182526	590940	12.16%	1.956%
44	23.957	3562	3569	3570	rBV2	95198	158315	3.26%	0.524%
45	23.992	3572	3575	3584	rVB3	136807	273217	5.62%	0.904%
46	24.433	3644	3650	3661	rVB	87143	246548	5.07%	0.816%
47	24.574	3668	3674	3682	rVB3	68856	180207	3.71%	0.596%
48	24.720	3689	3699	3709	rBV	591028	1649918	33.95%	5.461%
49	25.402	3810	3815	3824	rVB10	42105	101089	2.08%	0.335%
50	26.037	3915	3923	3932	rBV3	107931	331186	6.82%	1.096%
51	29.362	4481	4489	4490	rBV4	43707	86520	1.78%	0.286%
52	30.008	4591	4599	4616	rVB4	81812	367060	7.55%	1.215%

Sum of corrected areas: 30211971

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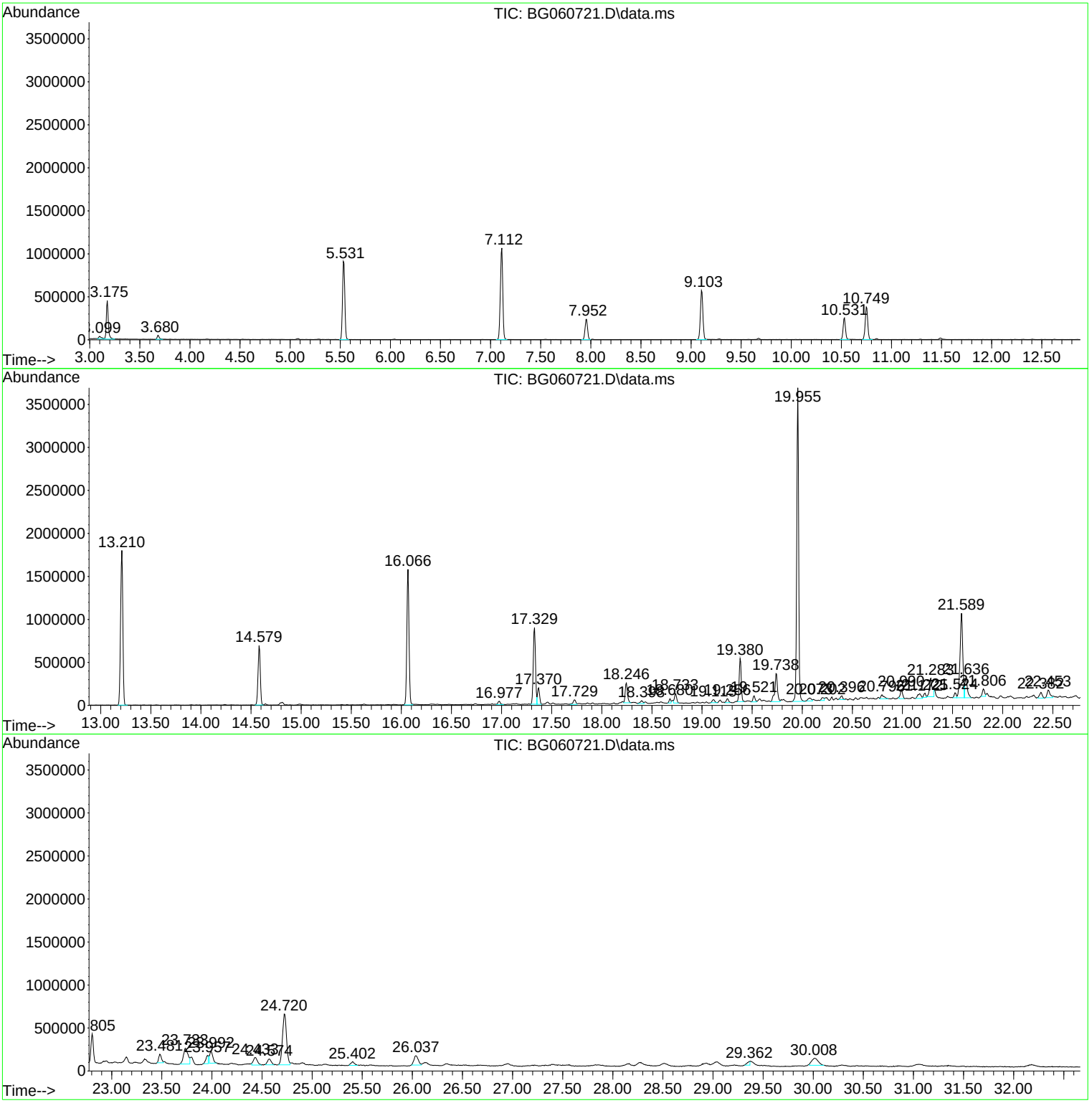
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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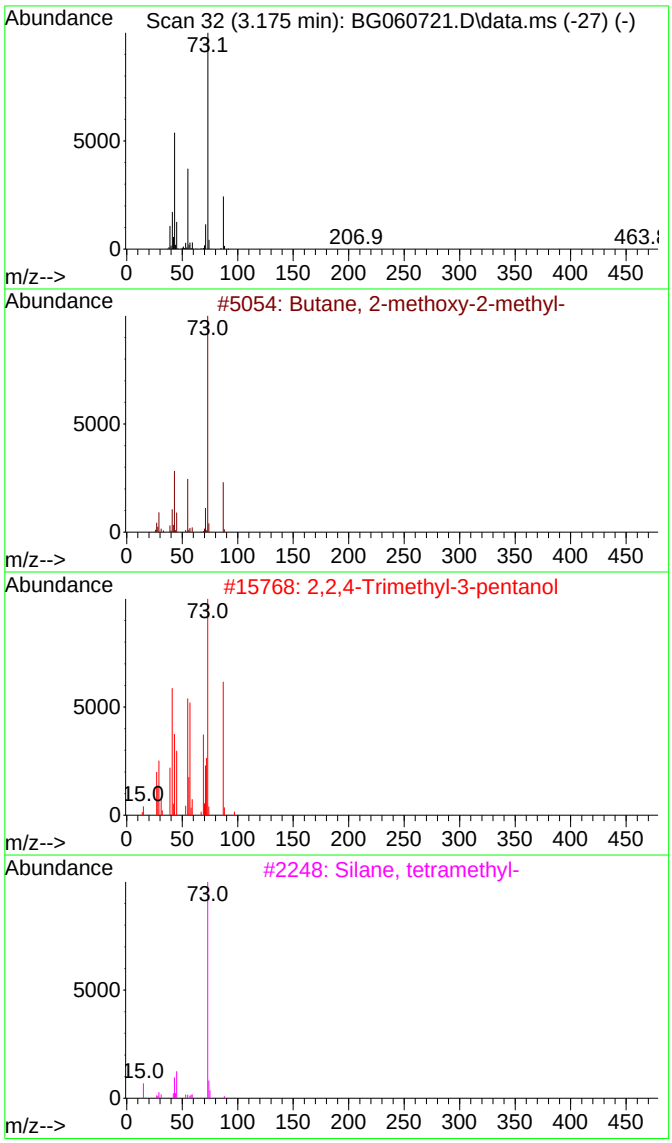
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

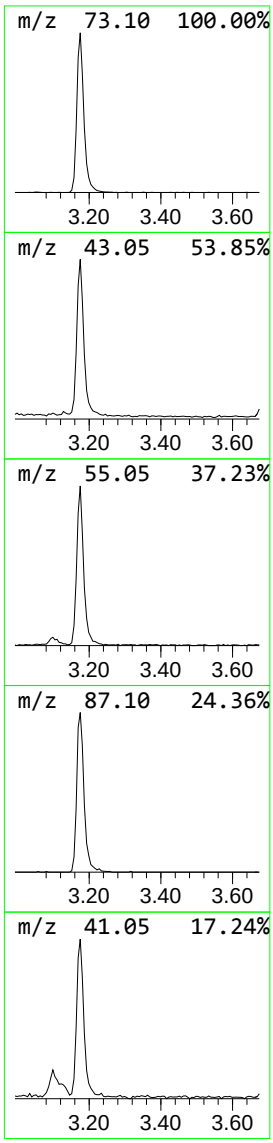
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.175	30.87 ng	624587	1,4-Dichlorobenzene-d4	7.958

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





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Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

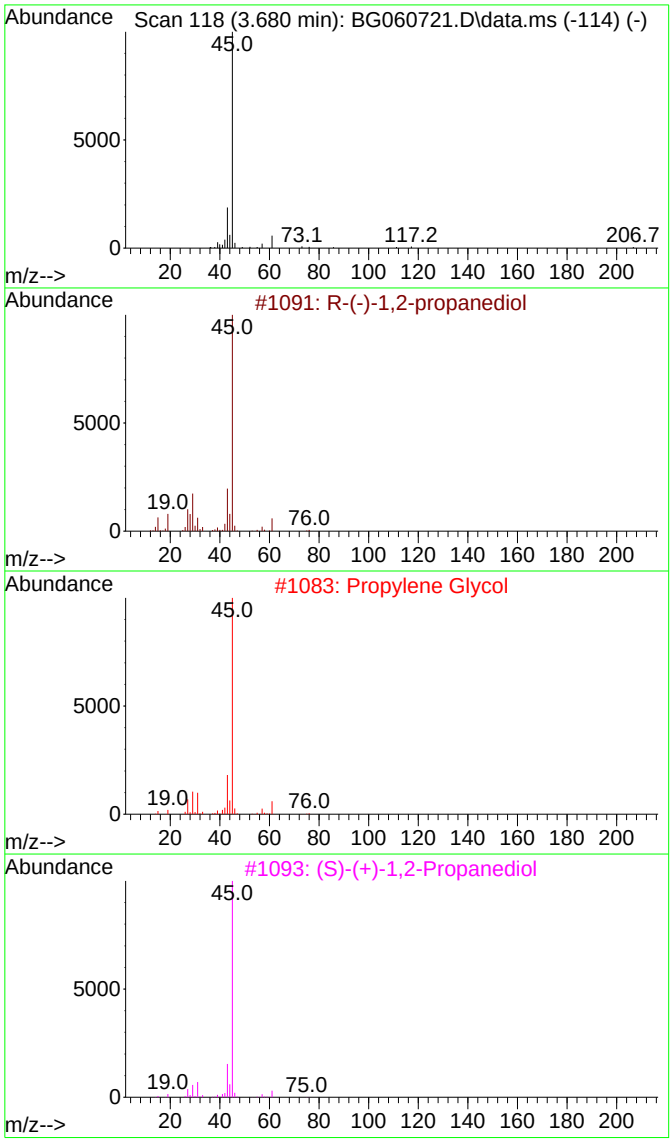
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

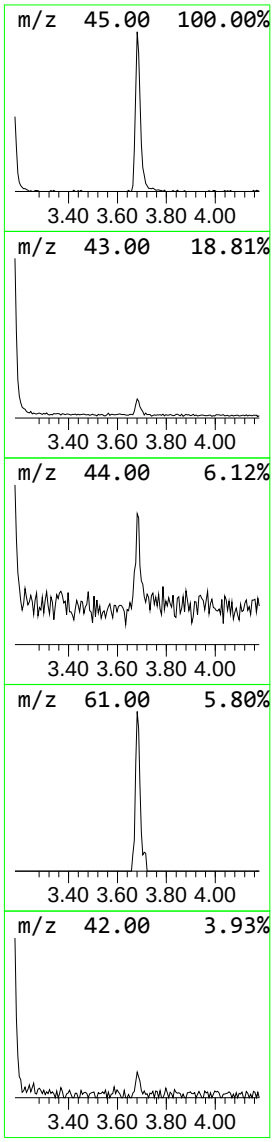
****

Peak Number 3 R-(-)-1,2-propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.680	3.17 ng	64124	1,4-Dichlorobenzene-d4	7.958

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
2	Propylene Glycol	76	C3H8O2	000057-55-6	72
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

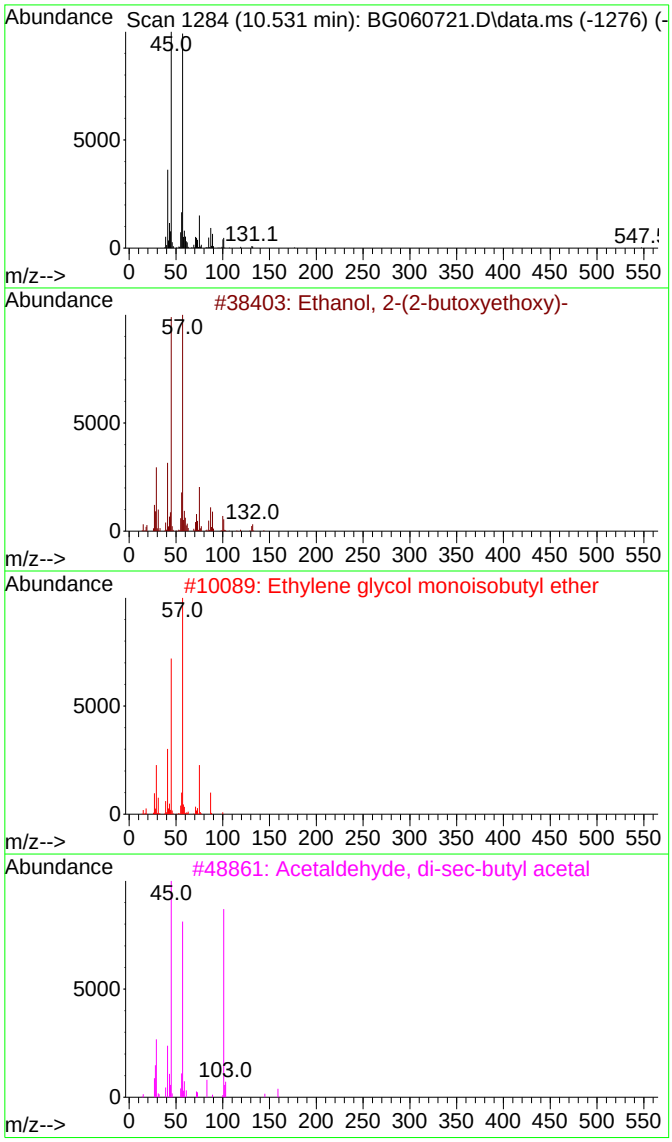
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

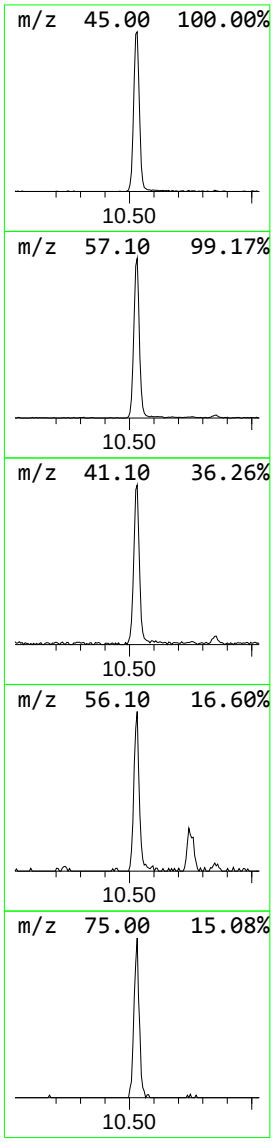
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.531	12.06 ng	403589	Naphthalene-d8	10.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53
4	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	53
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

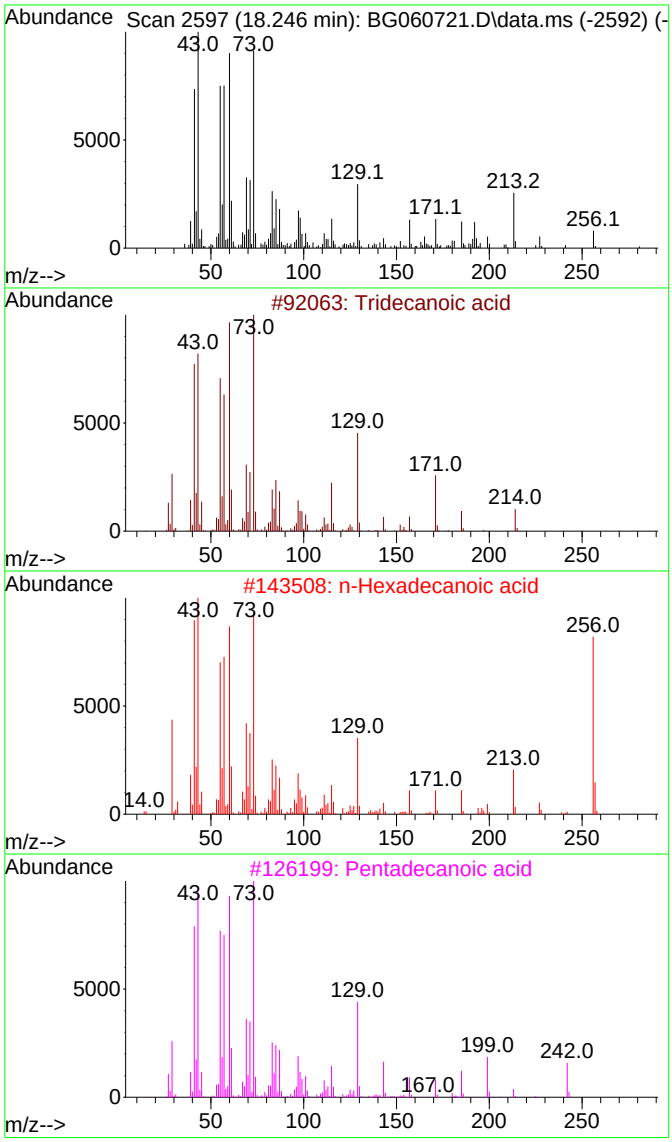
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

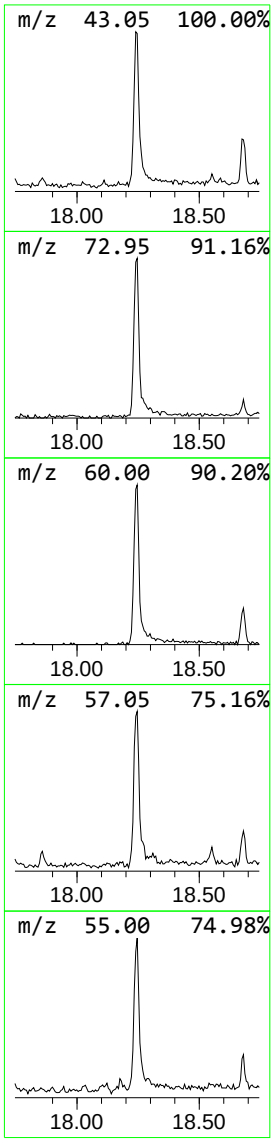
****

Peak Number 5 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.246	5.18 ng	355429	Phenanthrene-d10	17.329

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Undecanoic acid	186	C11H22O2	000112-37-8	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Sample : P1927-01
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

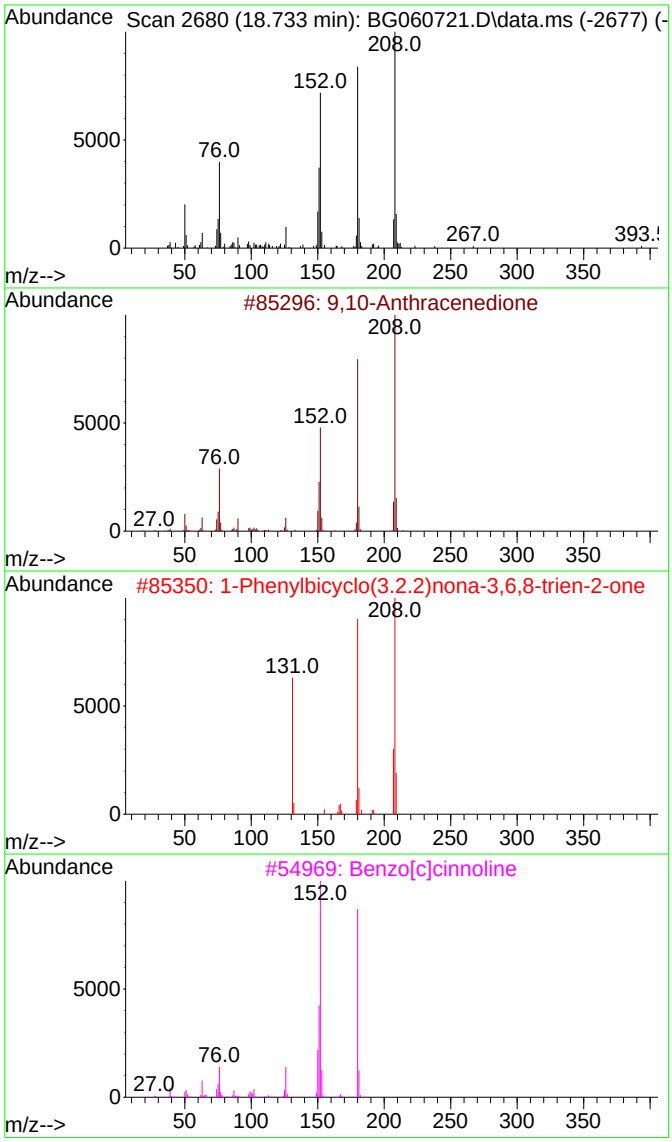
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

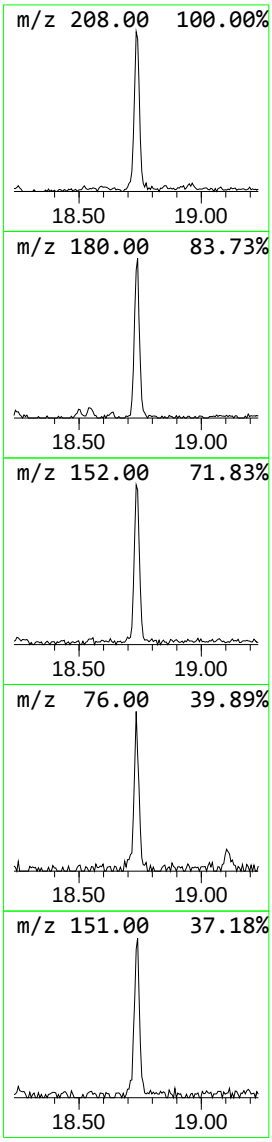
****

Peak Number 6 9,10-Anthracenedione Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.733	2.36 ng	161589	Phenanthrene-d10	17.329

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	96
2	1-Phenylbicyclo(3.2.2)nona-3,6,8...	208	C15H12O	1010427-19-9	58
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	55
4	9H-Fluoren-9-one	180	C13H8O	000486-25-9	55
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	49





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

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

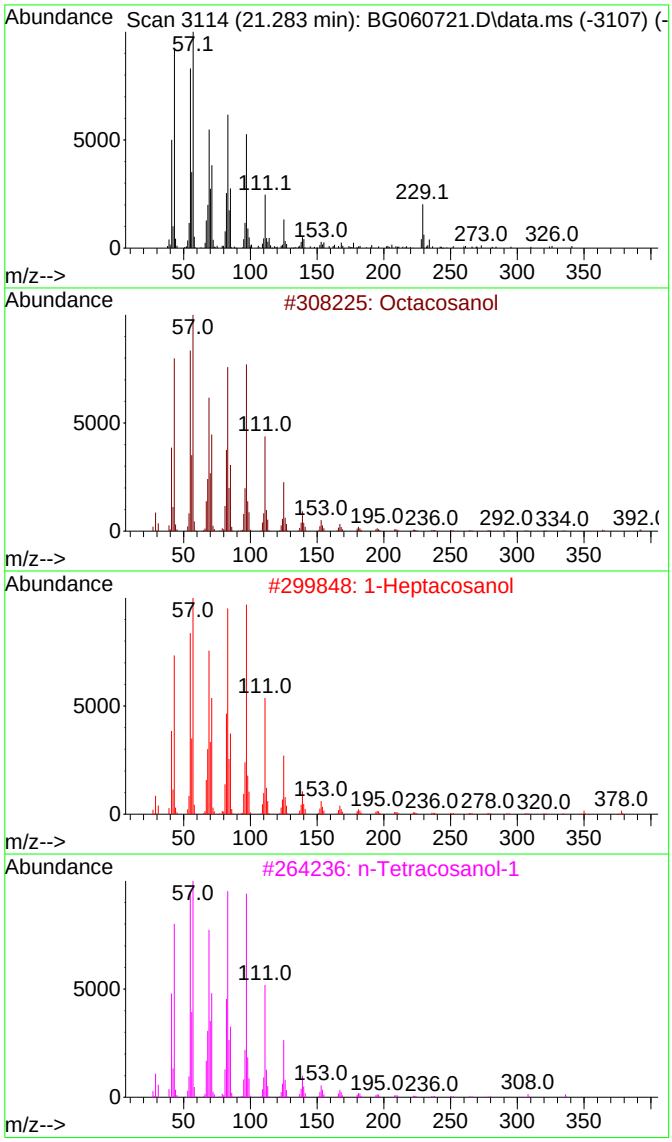
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

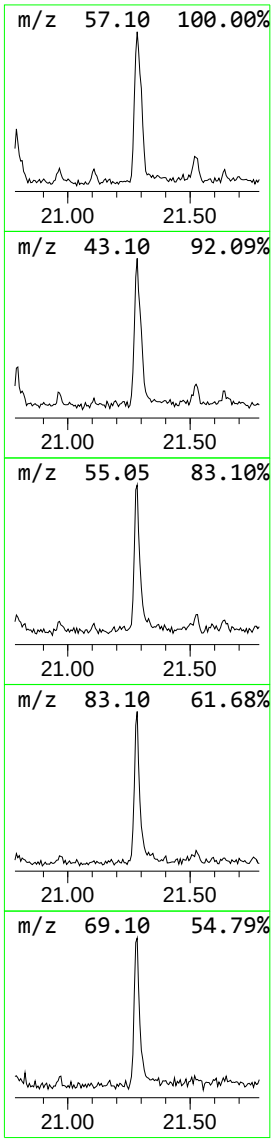
****

Peak Number 7 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.283	4.56 ng	429533	Chrysene-d12	21.589

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	81
2	1-Heptacosanol	396	C27H56O	002004-39-9	81
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	76
4	1-Hexacosanol	382	C26H54O	000506-52-5	76
5	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	74





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

Instrument :
BNA_G
ClientSampleId :
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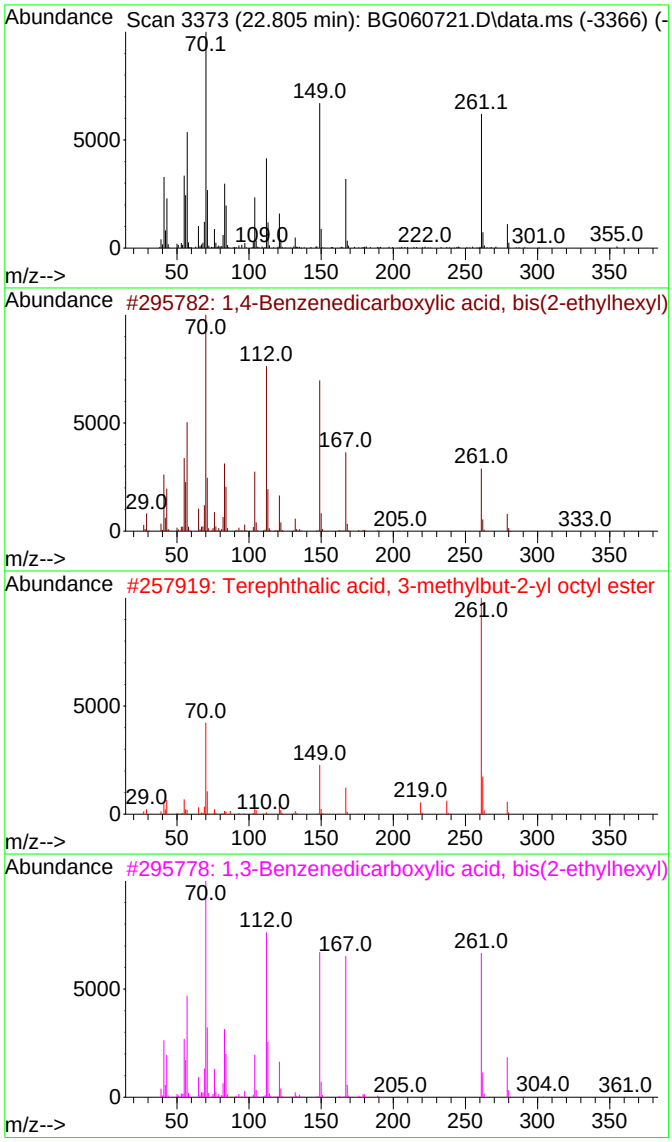
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

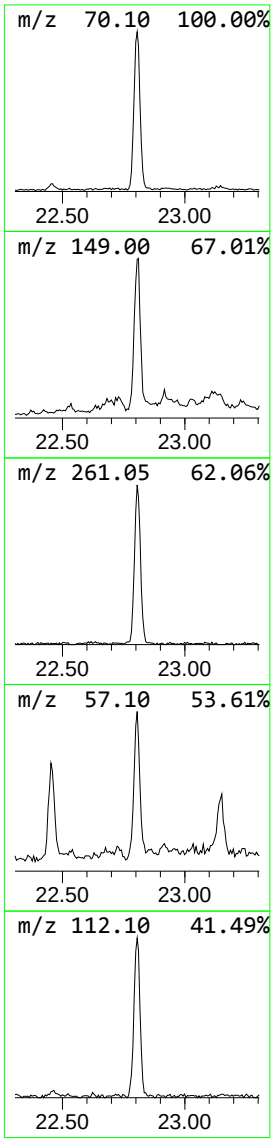
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.805	6.66 ng	626822	Chrysene-d12	21.589

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	76
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
4	Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	27
5	Acetic acid, [4-(4-methyl-1-pipe...	262	C14H18N2O3	346699-90-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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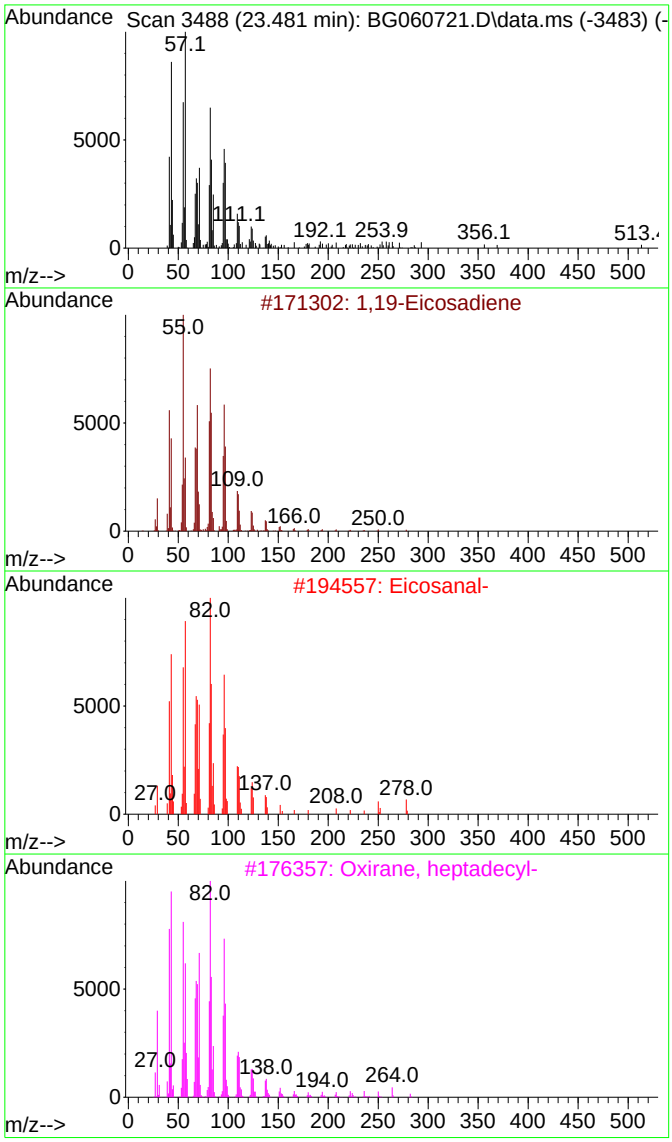
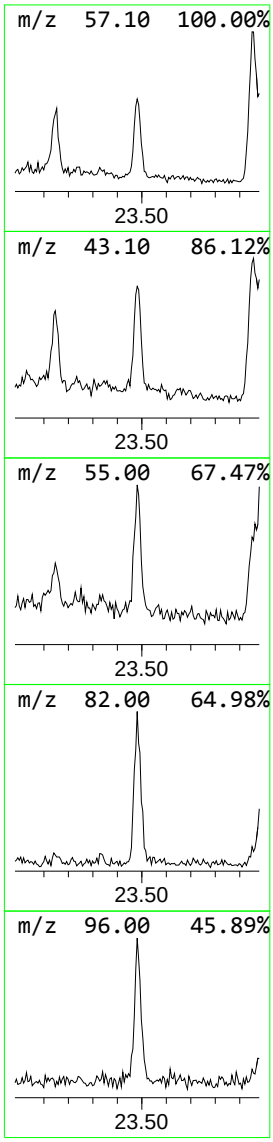
****

Peak Number 9 1,19-Eicosadiene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.481	2.29 ng	188583	Perylene-d12	24.720

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	90
2	Eicosanal-	296	C20H40O	002400-66-0	87
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5	Octadecanal	268	C18H36O	000638-66-4	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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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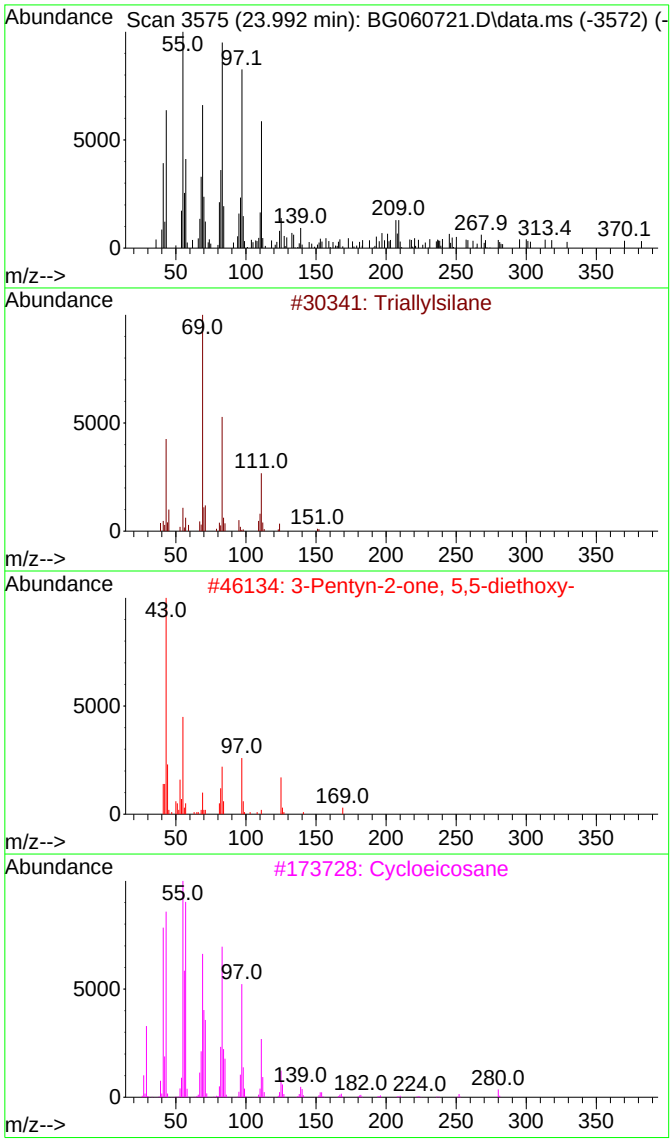
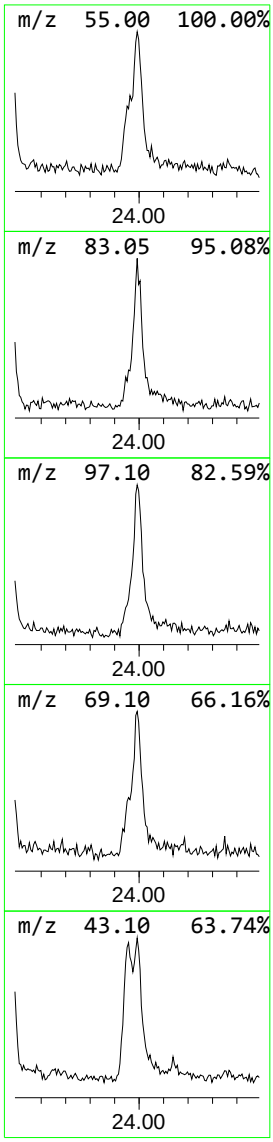
Peak Number 10 unknown23.992 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.992	3.31 ng	273217	Perylene-d12	24.720

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triallylsilane	152	C9H16Si	001116-62-7	43
2	3-Pentyn-2-one, 5,5-diethoxy-	170	C9H14O3	055402-04-5	43
3	Cycloeicosane	280	C20H40	000296-56-0	43
4	Muco-inositol tri-methaneboronate	252	C9H15B3O6	1000064-40-0	35
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	30





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Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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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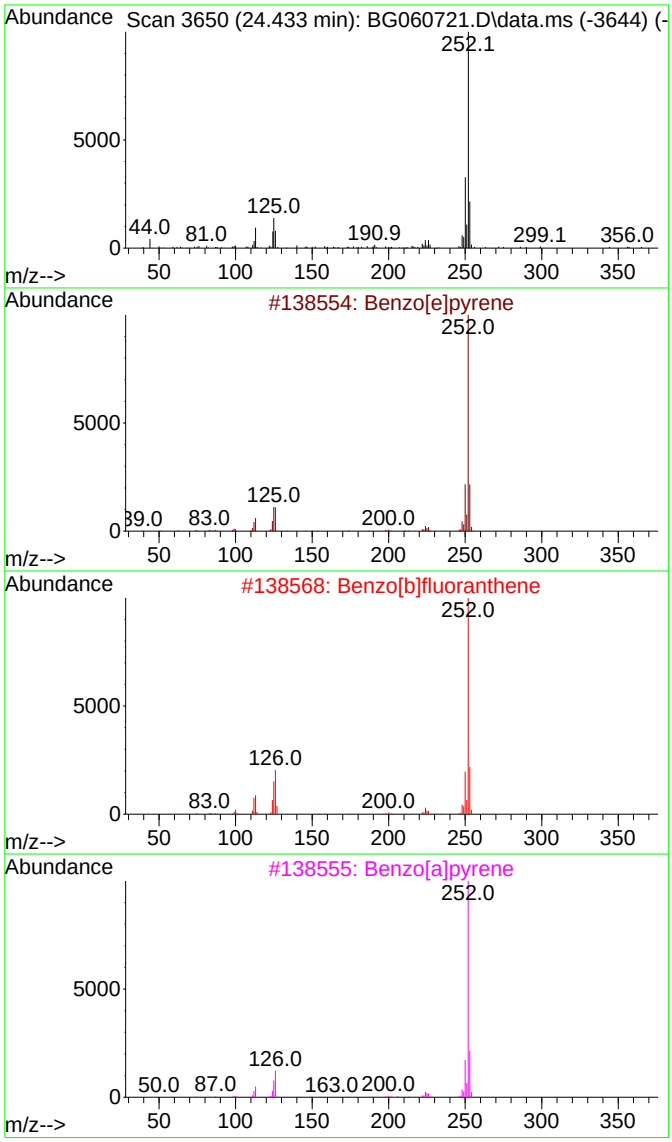
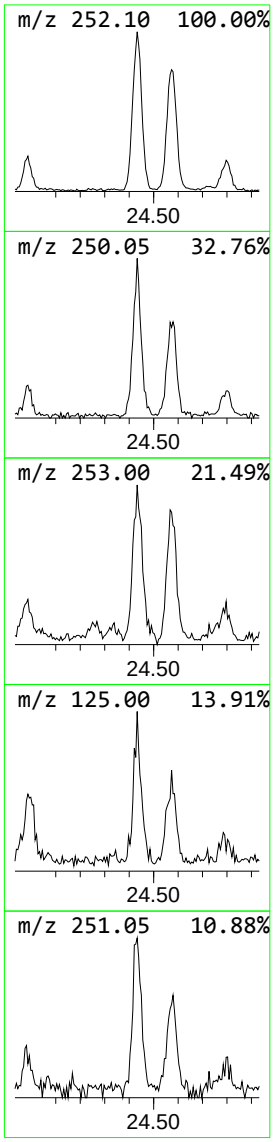
Peak Number 11 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.433	2.99 ng	246548	Perylene-d12	24.720

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	87
3	Benzo[a]pyrene	252	C20H12	000050-32-8	83
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	83
5	Perylene	252	C20H12	000198-55-0	74





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Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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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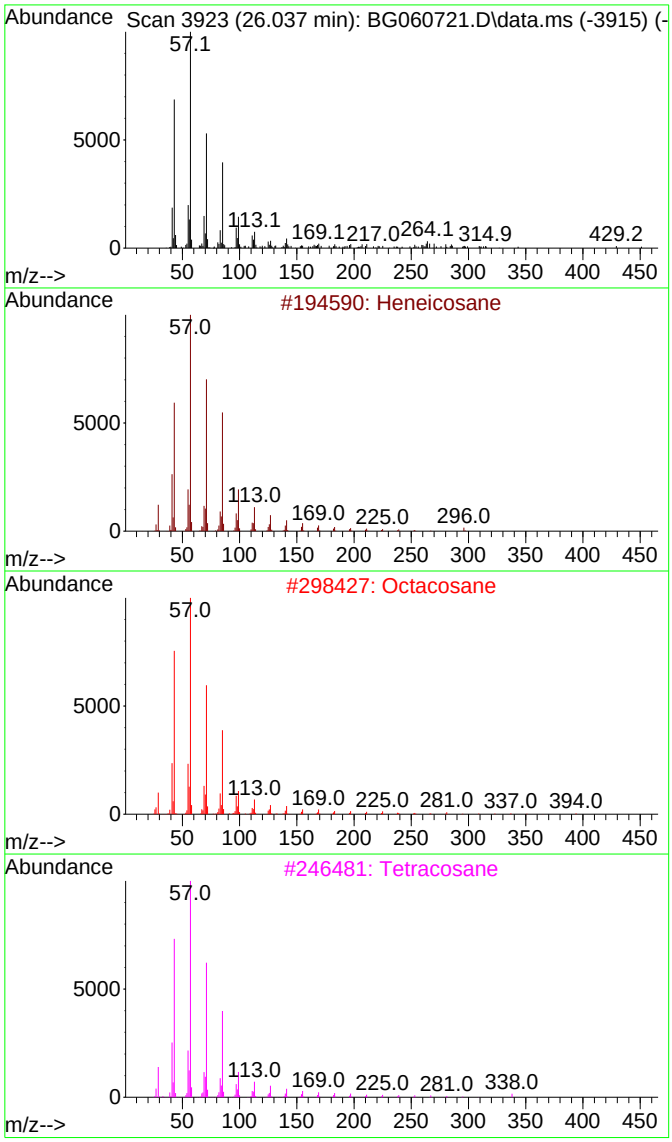
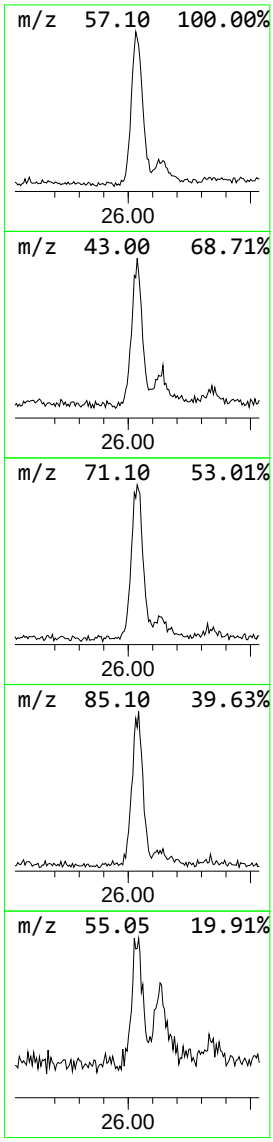
Peak Number 12 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.037	4.01 ng	331186	Perylene-d12	24.720

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Octacosane	394	C28H58	000630-02-4	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	86
5	Eicosane	282	C20H42	000112-95-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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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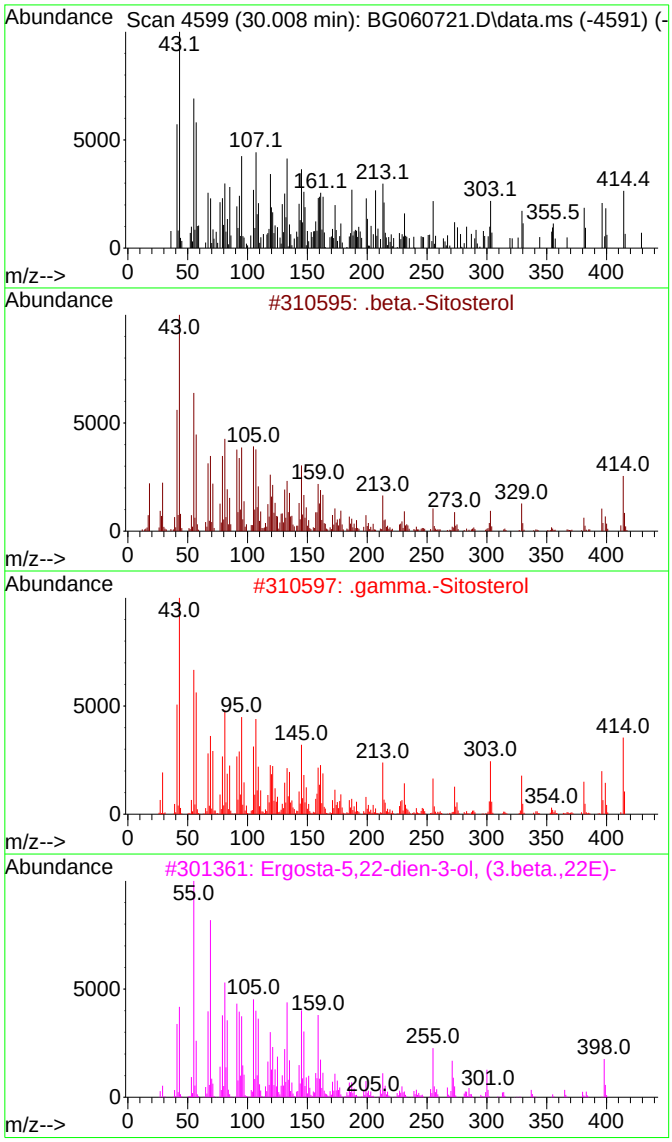
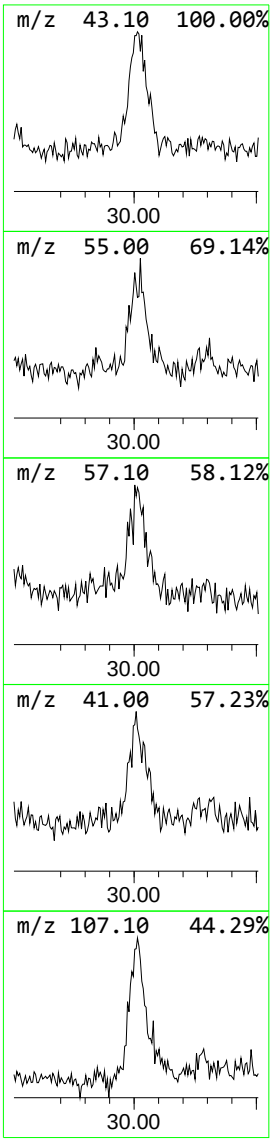
Peak Number 13 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.008	4.45 ng	367060	Perylene-d12	24.720

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	90
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	86
3	Ergosta-5,22-dien-3-ol, (3.beta....	398	C28H46O	000474-67-9	38
4	Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	38
5	(1S,2E,4E,7E,10R,11E)-10-Acetoxy...	330	C22H34O2	1000433-18-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060721.D
Acq On : 1 Apr 2024 18:53
Operator : MA/JU
Sample : P1927-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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...	3.175	30.9	ng	624587	1	7.958	404704	20.0
R-(-)-1,2-propa...	3.680	3.2	ng	64124	1	7.958	404704	20.0
Ethanol, 2-(2-b...	10.531	12.1	ng	403589	2	10.749	669201	20.0
Tridecanoic acid	18.246	5.2	ng	355429	4	17.329	1371520	20.0
9,10-Anthracene...	18.733	2.4	ng	161589	4	17.329	1371520	20.0
Octacosanol	21.283	4.6	ng	429533	5	21.589	1883560	20.0
1,4-Benzenedica...	22.805	6.7	ng	626822	5	21.589	1883560	20.0
1,19-Eicosadiene	23.481	2.3	ng	188583	6	24.720	1649920	20.0
unknown23.992	23.992	3.3	ng	273217	6	24.720	1649920	20.0
Benzo[e]pyrene	24.433	3.0	ng	246548	6	24.720	1649920	20.0
Heneicosane	26.037	4.0	ng	331186	6	24.720	1649920	20.0
.beta.-Sitosterol	30.008	4.5	ng	367060	6	24.720	1649920	20.0