LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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: BG060720.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.102	14	19	26	rVV3	32434	59657	1.51%	0.230%
2	3.172	26	31	43	rVB	470422	645032	16.36%	2.482%
3	3.684	113	118	127	rVB	57358	84850	2.15%	0.327%
4	5.534	425	433	443	rBV	974025	1484242	37.65%	5.712%
5	7.109	693	701	712	rBV	911966	1517685	38.50%	5.841%
6	7.955	838	845	851	rBV	231295	385314	9.77%	1.483%
7	9.107	1032	1041	1050	rBV	477976	835877	21.20%	3.217%
8	10.529	1276	1283	1290	rBV	131696	207950	5.28%	0.800%
9	10.752	1312	1321	1332	rBV	360186	632434	16.04%	2.434%
10	11.486	1441	1446	1452	rBV2	21874	39918	1.01%	0.154%
11	13.208	1732	1739	1748	rVB	1494479	2286642	58.01%	8.800%
12	14.583	1965	1973	1979	rBV	671496	1033193	26.21%	3.976%
13	14.982	2035	2041	2050	rVB2	38959	67798	1.72%	0.261%
14	15.628	2143	2151	2157	rBV	49778	71989	1.83%	0.277%
15	16.063	2219	2225	2235	rBV	1311631	1963964	49.82%	7.558%
16	16.292	2256	2264	2272	rBV4	30290	66028	1.68%	0.254%
17	16.974	2375	2380	2390	rVB	134443	208931	5.30%	0.804%
18	17.326	2434	2440	2444	rBV	872041	1342350	34.05%	5.166%
19	17.368	2444	2447	2453	rVB	420328	591405	15.00%	2.276%
20	17.456	2459	2462	2469	rVB	55389	82496	2.09%	0.317%
21	17.726	2500	2508	2512	rBV2	50918	97462	2.47%	0.375%
22	18.208	2586	2590	2592	rBV	33860	41532	1.05%	0.160%
23	18.243	2592	2596	2605	rVB2	262587	394809	10.02%	1.519%
24	18.396	2616	2622	2627	rBV4	47010	85582	2.17%	0.329%
25	18.737	2677	2680	2686	rVB	45440	66074	1.68%	0.254%
26	19.048	2729	2733	2738	rVB7	32506	42974	1.09%	0.165%
27	19.107	2739	2743	2750	rBV4	46468	87802	2.23%	0.338%
28	19.377	2784	2789	2798	rBV	313974	503938	12.78%	1.939%
29	19.518	2809	2813	2818	rBV2	71210	85829	2.18%	0.330%
30	19.741	2842	2851	2858	rBV2	211040	433203	10.99%	1.667%
31	19.953	2879	2887	2898	rVB	2919900	3941890	100.00%	15.170%
32	20.070	2902	2907	2908	rBV4	24804	42647	1.08%	0.164%
33	20.111	2911	2914	2918	rVB3	39936	53790	1.36%	0.207%
34	20.294	2942	2945	2949	rVB2	38881	42471	1.08%	0.163%
35	20.487	2974	2978	2982	rVB3	57516	75282	1.91%	0.290%
36	20.793	3027	3030	3033	rVB	42796	45227	1.15%	0.174%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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	21.228	3100	3104	3107	rBV5	41466	67915	1.72%	0.261%
38	21.281	3109	3113	3129	rVB4	190884	433809	11.01%	1.670%
39	21.527	3151	3155	3158	rBV4	36059	50795	1.29%	0.195%
40	21.586	3158	3165	3171	rBV	876253	1563721	39.67%	6.018%
41	21.845	3206	3209	3214	rVB2	43002	53651	1.36%	0.206%
42	22.456	3309	3313	3317	rBV3	59553	92635	2.35%	0.357%
43	22.808	3366	3373	3385	rBV	1078314	2017239	51.17%	7.763%
44	23.337	3457	3463	3473	rVB4	73036	204499	5.19%	0.787%
45	23.954	3564	3568	3580	rVB6	44439	114927	2.92%	0.442%
46	24.724	3689	3699	3716	rBV	561524	1613420	40.93%	6.209%
47	26.040	3917	3923	3932	rVB3	44393	123211	3.13%	0.474%

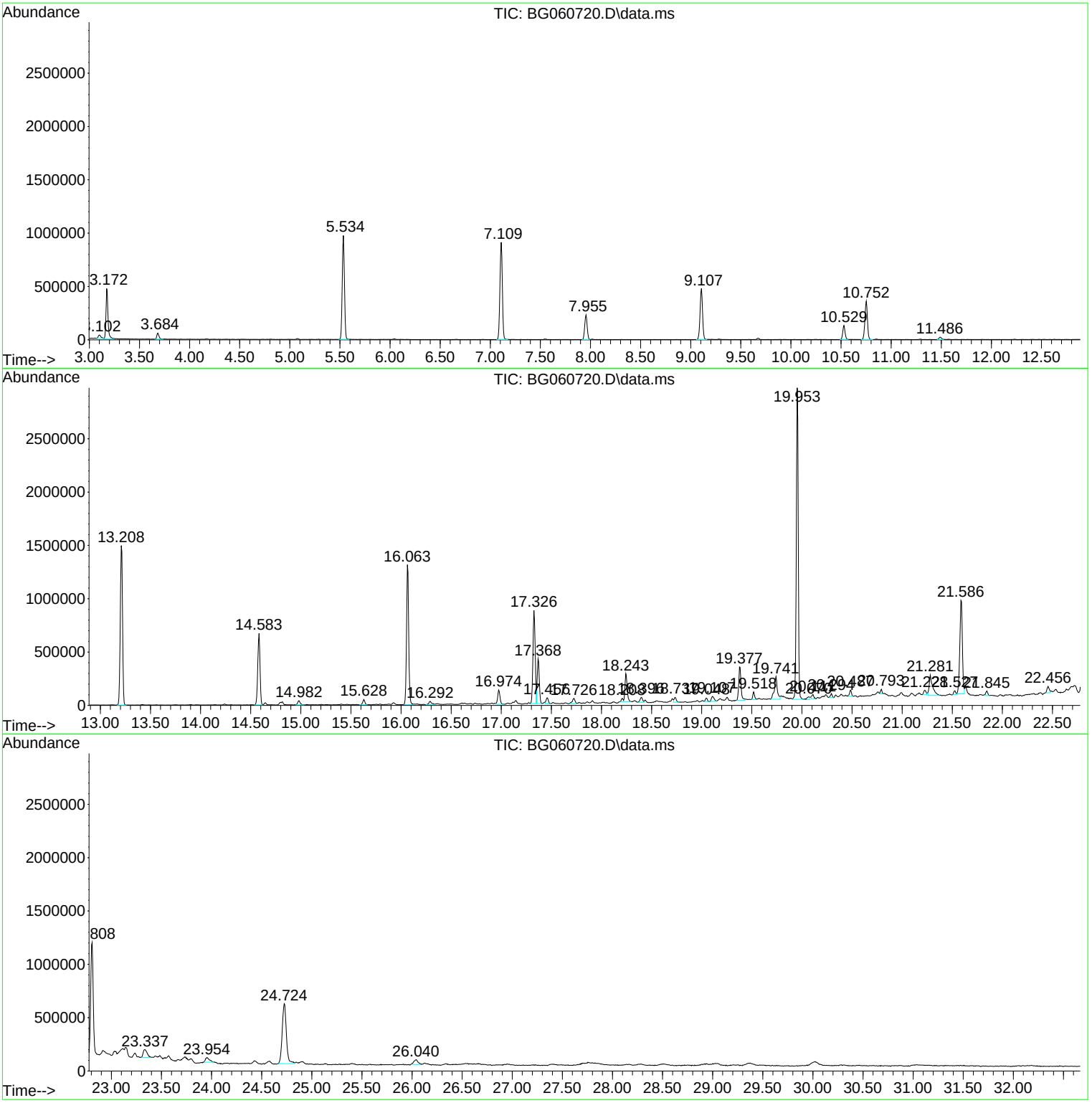
Sum of corrected areas: 25984089

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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 : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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

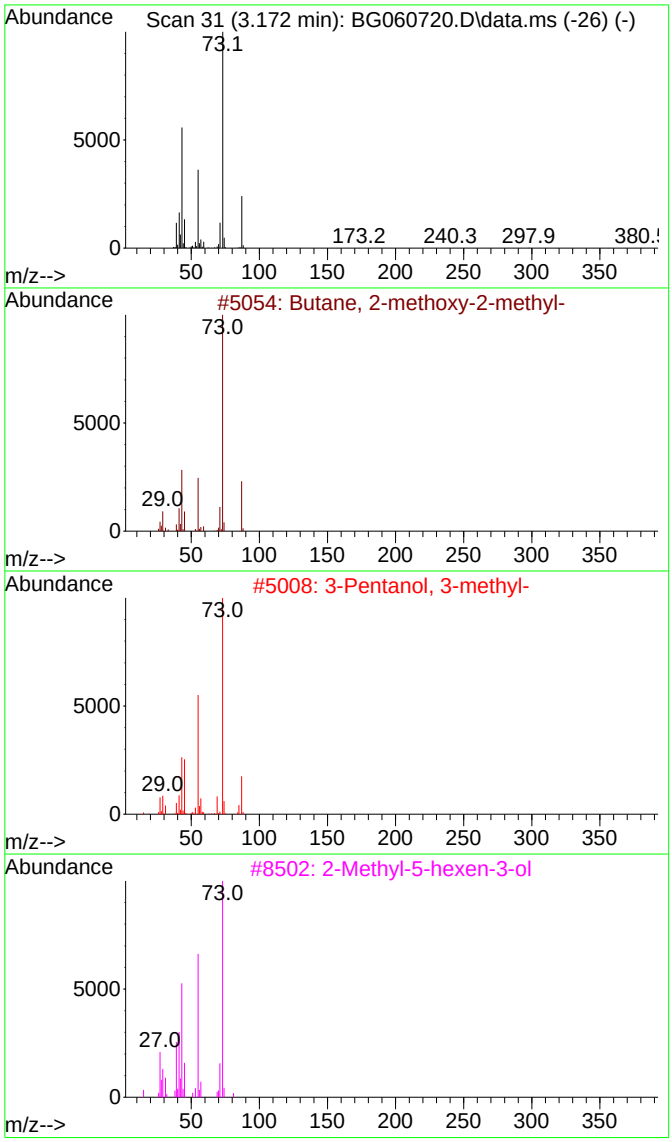
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

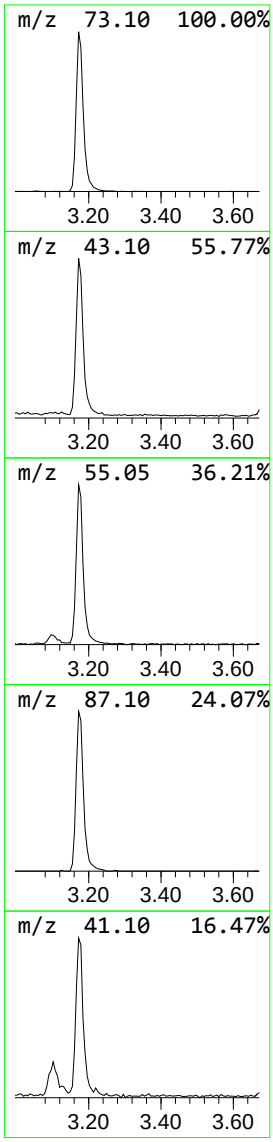
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.172	33.48 ng	645032	1,4-Dichlorobenzene-d4	7.955

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	45
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	43
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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

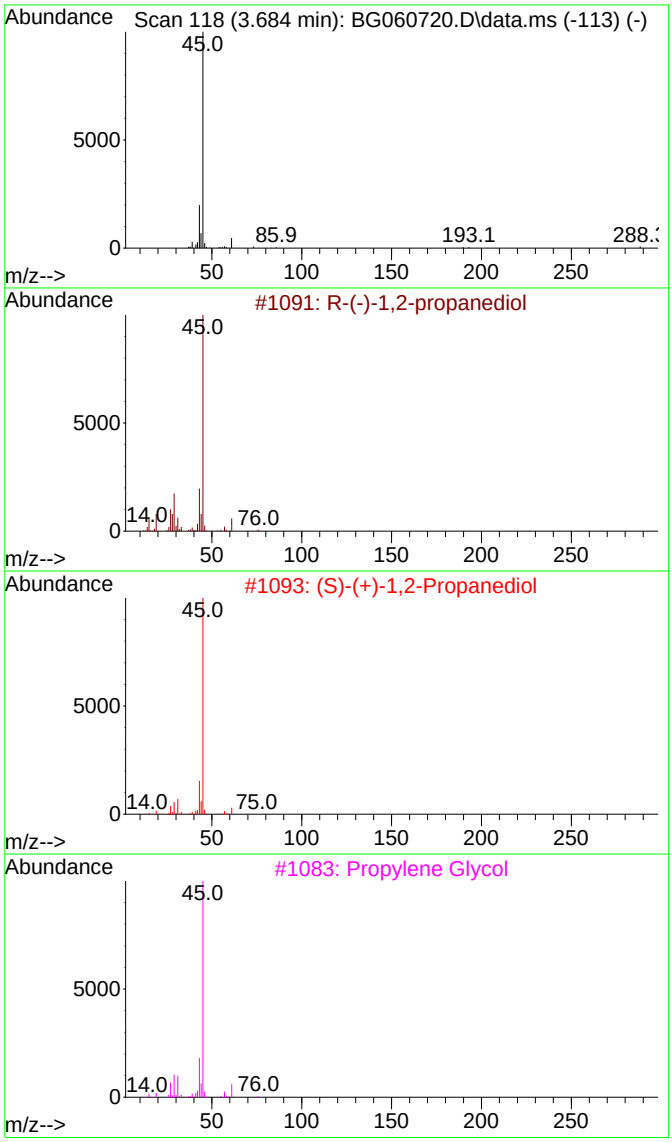
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

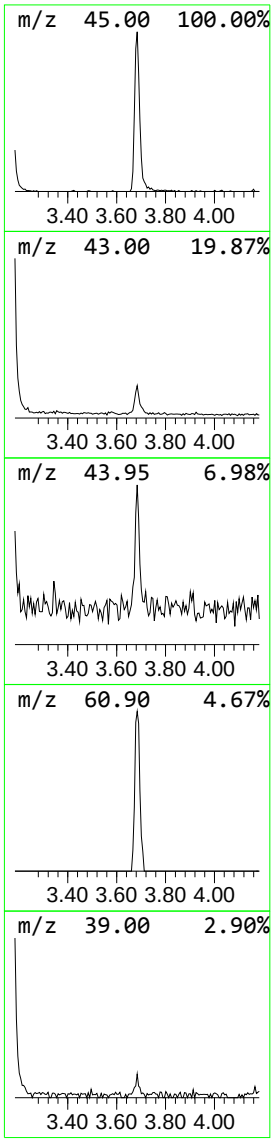
****

Peak Number 3 unknown3.684 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.684	4.40 ng	84850	1,4-Dichlorobenzene-d4	7.955

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3	Propylene Glycol	76	C3H8O2	000057-55-6	40
4	Ethane, 1,1-diethoxy-	118	C6H14O2	000105-57-7	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

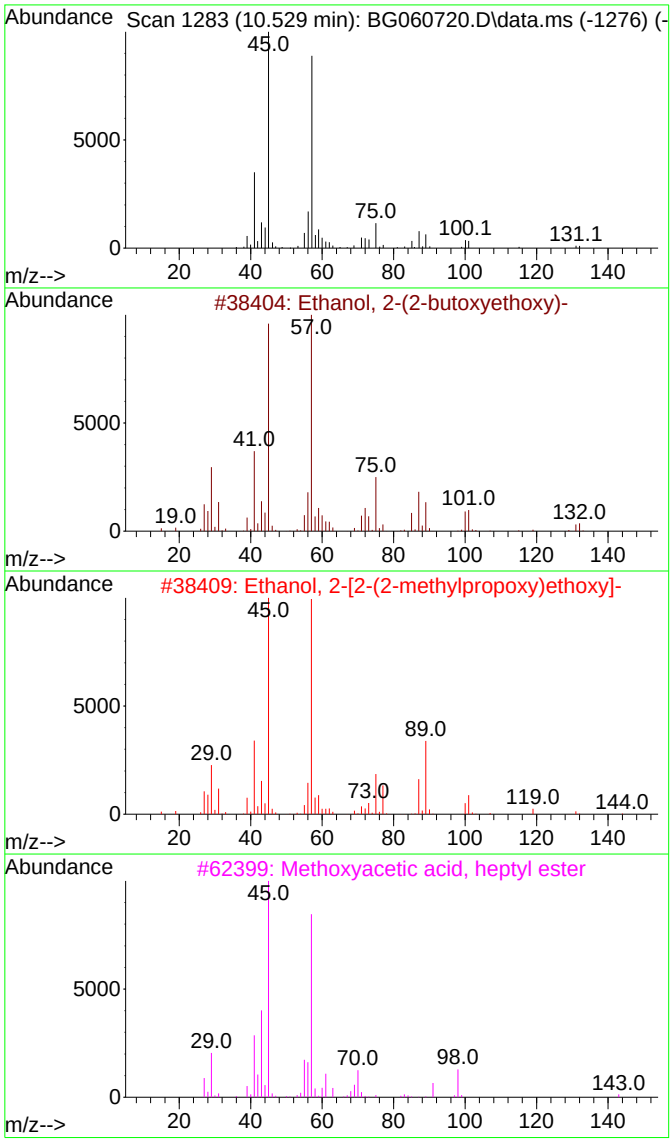
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

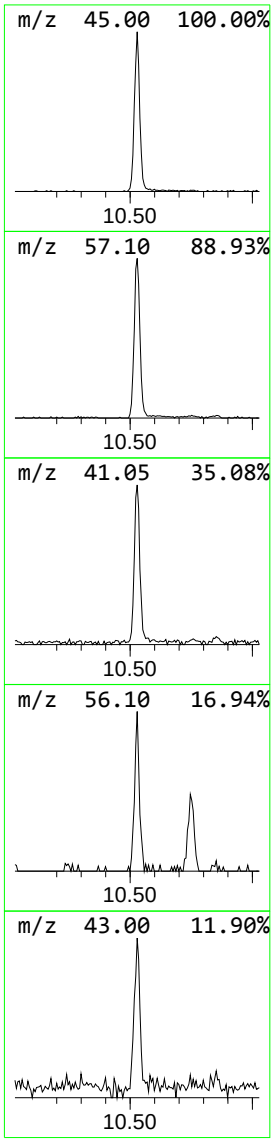
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.529	6.58 ng	207950	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	53
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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

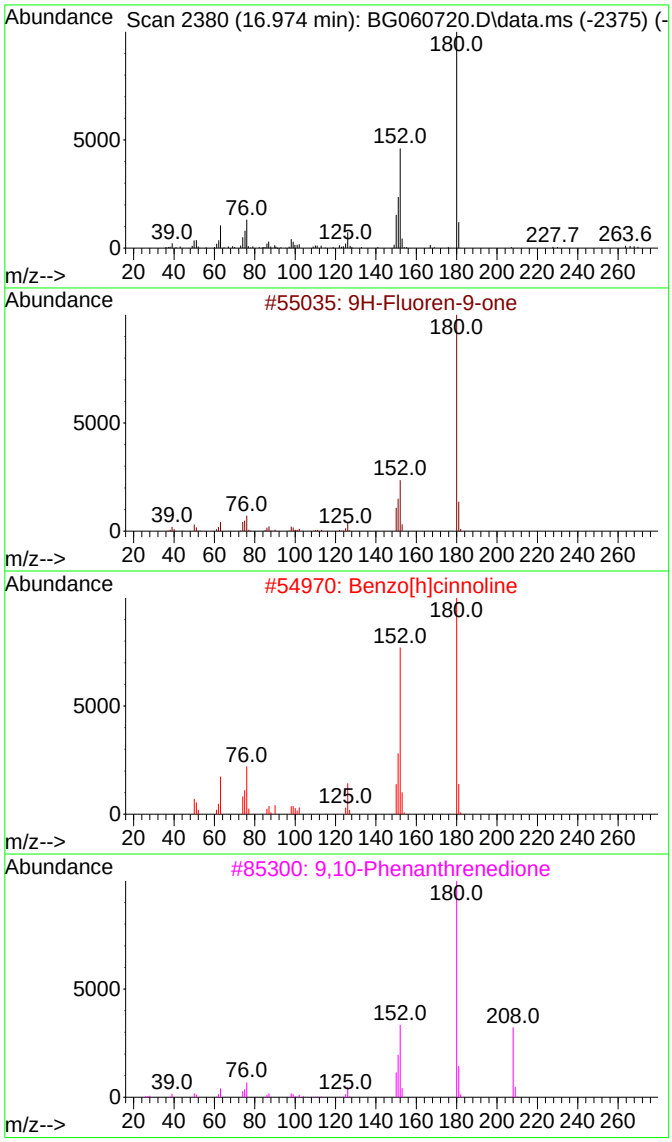
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

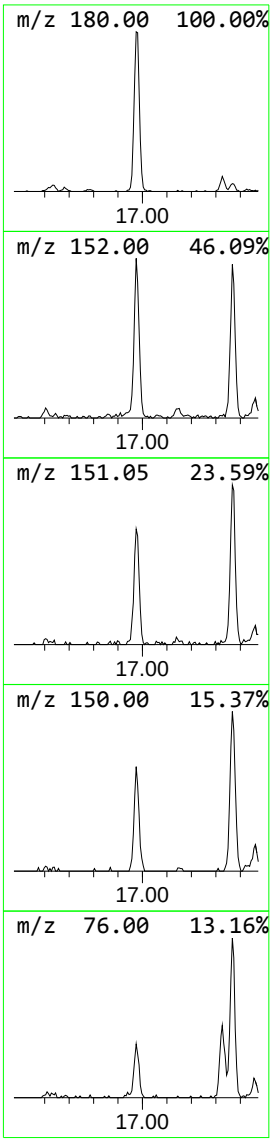
****

Peak Number 5 9H-Fluoren-9-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.974	3.11 ng	208931	Phenanthrene-d10	17.326

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluoren-9-one	180	C13H8O	000486-25-9	95
2	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	90
3	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	83
4	Diphenic anhydride	224	C14H8O3	006050-13-1	64
5	2,3-Diazaphenanthrene	180	C12H8N2	000229-72-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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

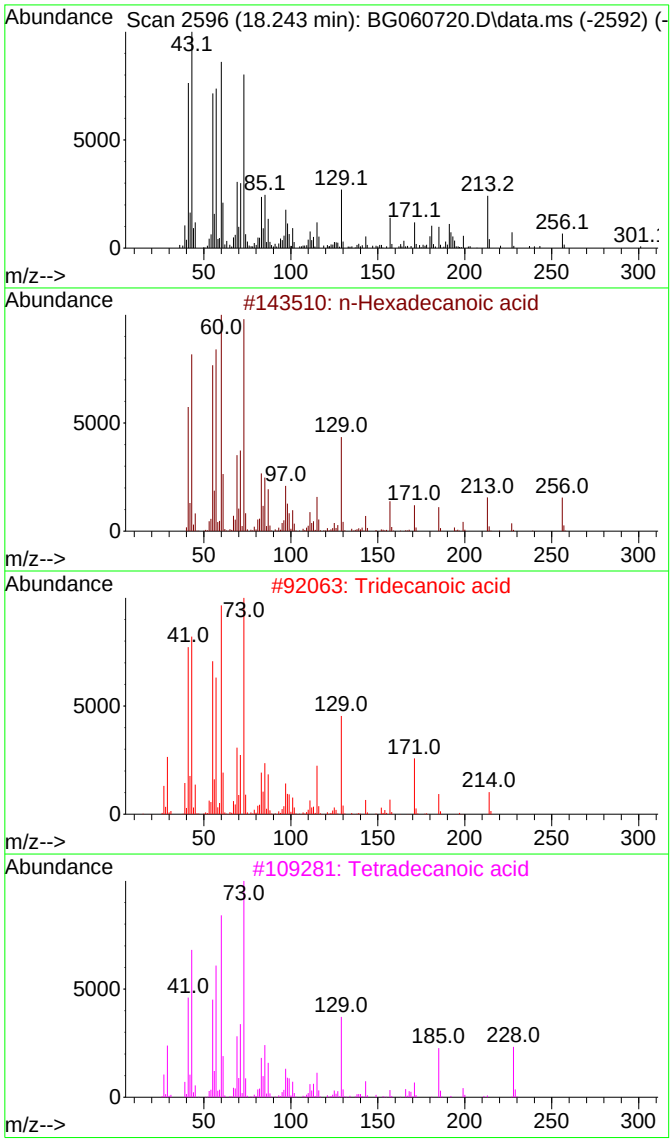
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

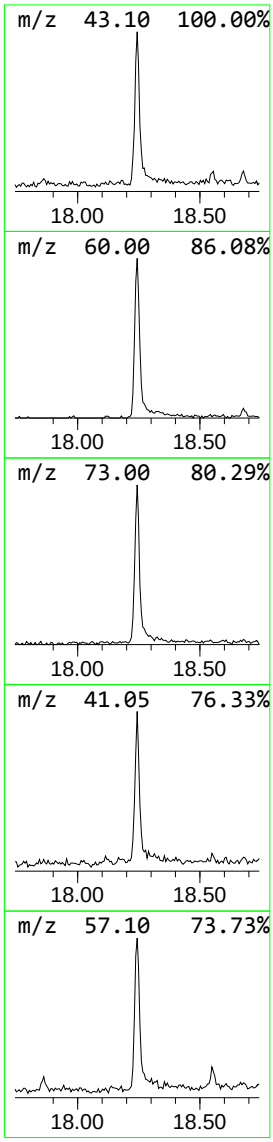
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.243	5.88 ng	394809	Phenanthrene-d10	17.326

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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

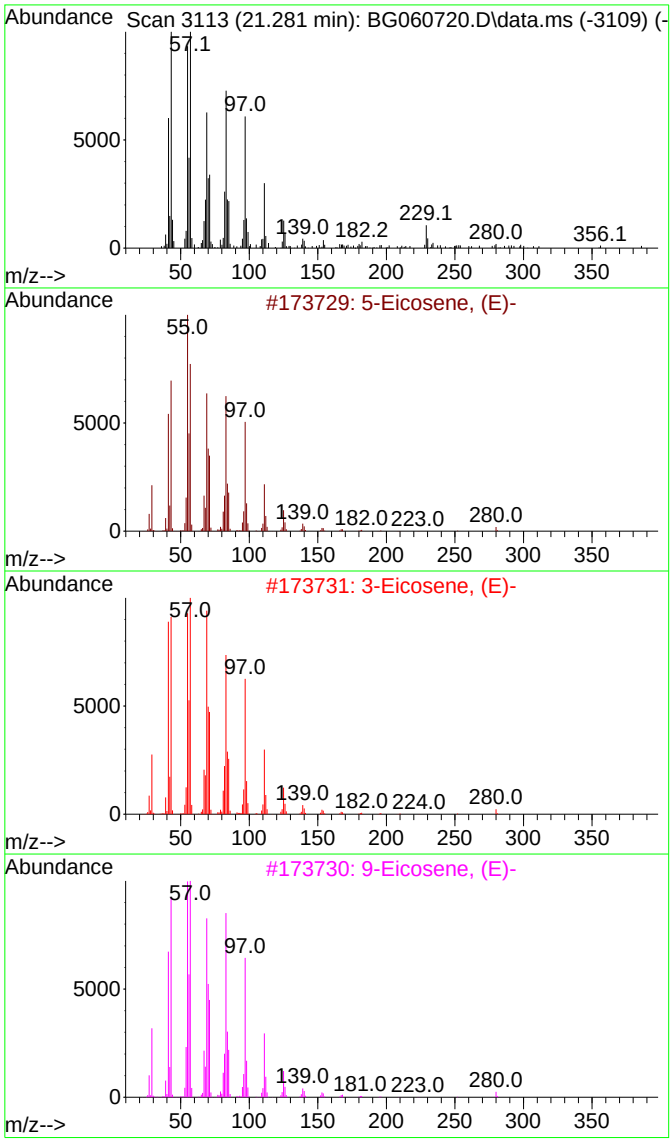
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

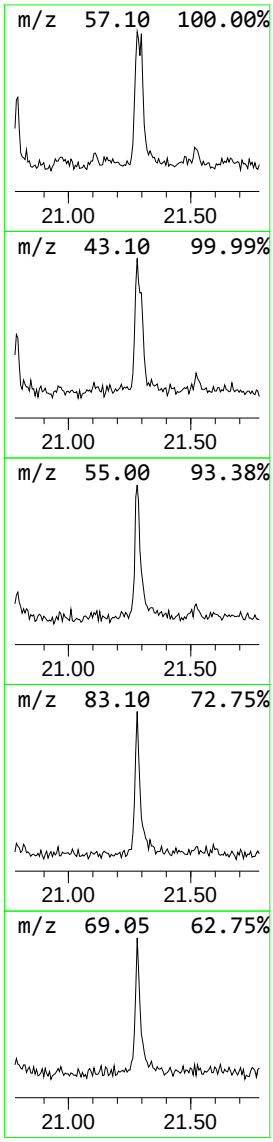
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.281	5.55 ng	433809	Chrysene-d12	21.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4	cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	93
5	1-Docosene	308	C22H44	001599-67-3	90





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Data File : BG060720.D
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Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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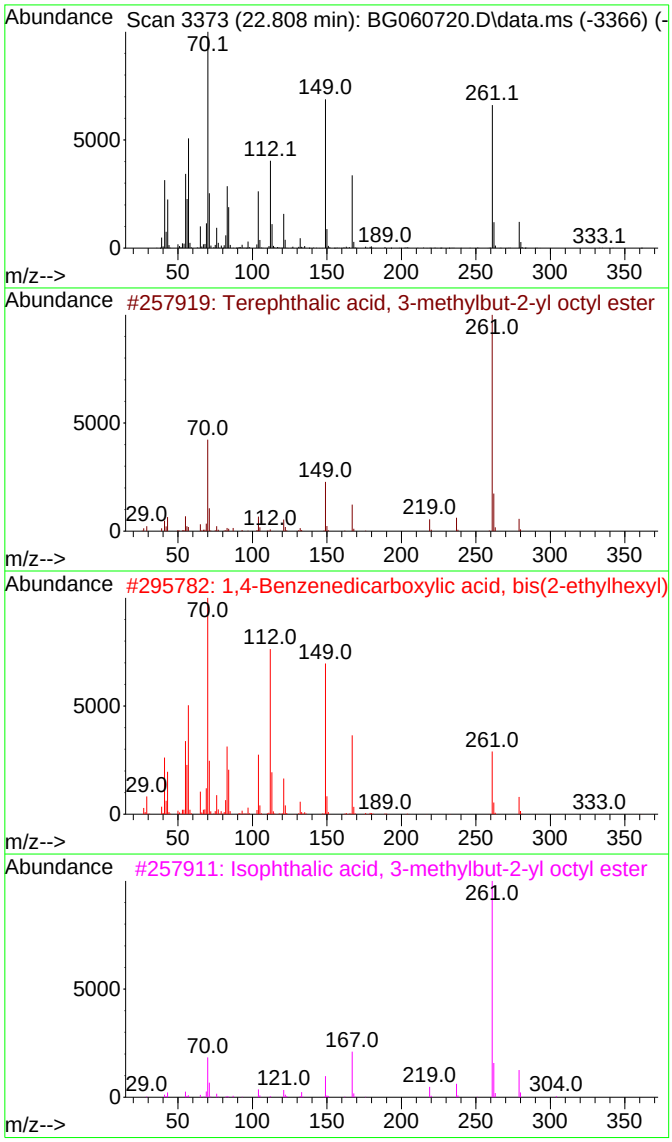
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

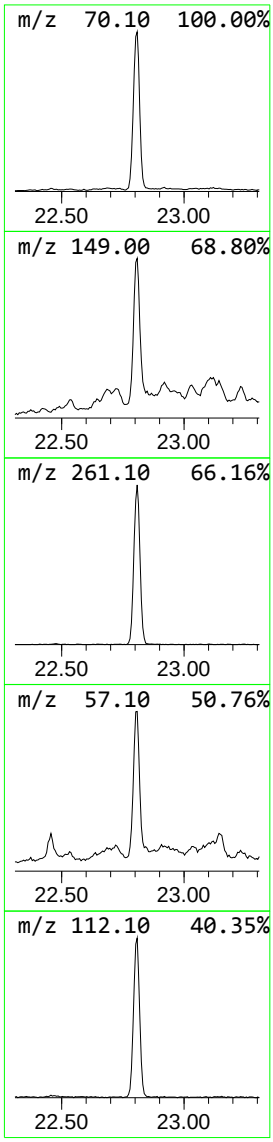
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Terephthalic acid, 3-methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.808	25.80 ng	2017240	Chrysene-d12	21.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
3	Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	50
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
5	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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

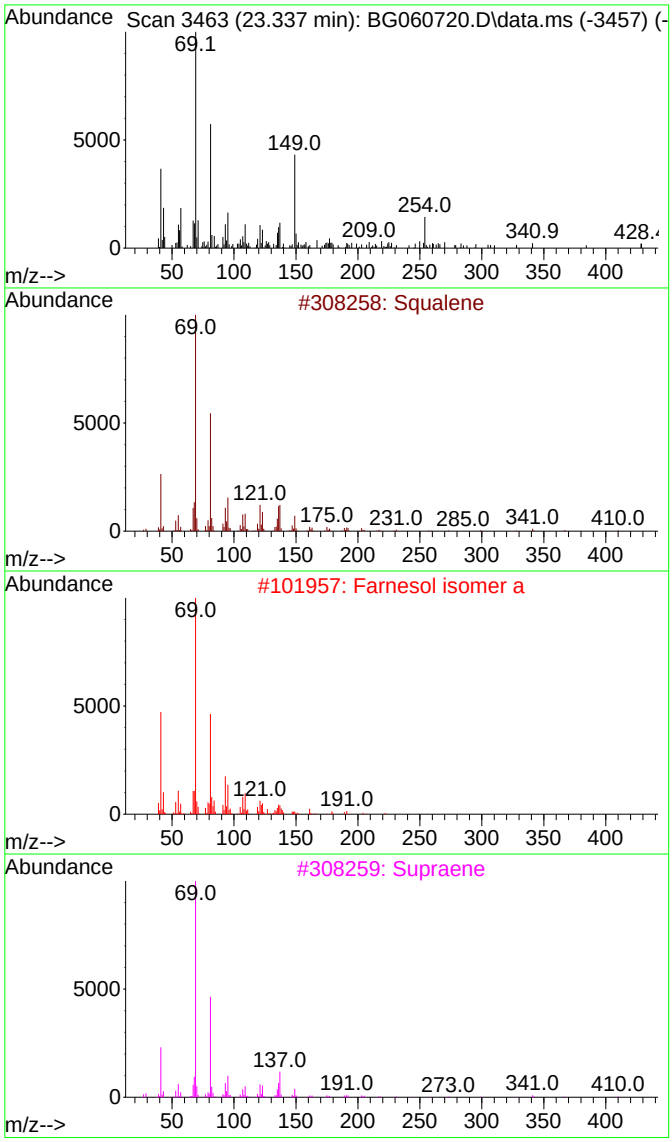
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

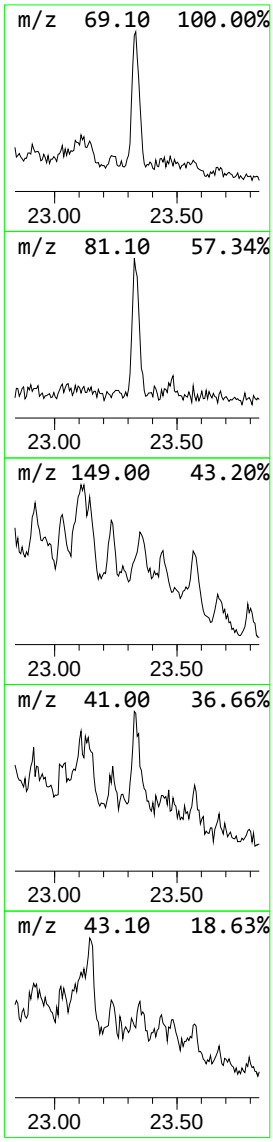
****

Peak Number 9 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.337	2.53 ng	204499	Perylene-d12	24.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	70
2	Farnesol isomer a	222	C15H26O	1000108-92-4	58
3	Supraene	410	C30H50	007683-64-9	58
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	52
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060720.D
Acq On : 1 Apr 2024 18:12
Operator : MA/JU
Sample : P1927-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11998

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...	3.172	33.5	ng	645032	1	7.955	385314	20.0
unknown3.684	3.684	4.4	ng	84850	1	7.955	385314	20.0
Ethanol, 2-(2-b...	10.529	6.6	ng	207950	2	10.752	632434	20.0
9H-Fluoren-9-one	16.974	3.1	ng	208931	4	17.326	1342350	20.0
n-Hexadecanoic ...	18.243	5.9	ng	394809	4	17.326	1342350	20.0
5-Eicosene, (E)-	21.281	5.5	ng	433809	5	21.586	1563720	20.0
Terephthalic ac...	22.808	25.8	ng	2017240	5	21.586	1563720	20.0
Squalene	23.337	2.5	ng	204499	6	24.724	1613420	20.0