LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012224\
Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CHRT-24376

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-BG010824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.646	89	95	110	rBV	1542605	2498970	26.68%	3.106%
2	5.503	404	411	431	rBV	2498939	4147061	44.27%	5.154%
3	7.095	674	682	699	rBV	2335159	4018628	42.90%	4.994%
4	7.929	816	824	840	rBV	1463913	2489283	26.57%	3.094%
5	9.093	1015	1022	1031	rBV	1503967	2694345	28.76%	3.348%
6	10.732	1288	1301	1311	rBV	2181957	4082538	43.58%	5.074%
7	11.425	1415	1419	1426	rVB8	109771	214250	2.29%	0.266%
8	11.831	1484	1488	1493	rVB5	118842	225734	2.41%	0.281%
9	11.919	1499	1503	1509	rVB6	138646	230111	2.46%	0.286%
10	12.459	1591	1595	1601	rBV7	132054	265295	2.83%	0.330%
11	12.641	1622	1626	1631	rBV2	255581	391087	4.17%	0.486%
12	13.006	1685	1688	1693	rVB4	205901	291376	3.11%	0.362%
13	13.188	1710	1719	1728	rBV	4108235	6806455	72.66%	8.459%
14	13.270	1729	1733	1738	rBV7	207439	370458	3.95%	0.460%
15	13.347	1742	1746	1749	rBV6	428741	682247	7.28%	0.848%
16	13.834	1826	1829	1835	rBV6	445166	867506	9.26%	1.078%
17	13.916	1839	1843	1851	rVB	1091549	2016275	21.52%	2.506%
18	13.987	1852	1855	1859	rBV3	721661	1083201	11.56%	1.346%
19	14.310	1906	1910	1915	rBV7	651508	1489129	15.90%	1.851%
20	14.398	1921	1925	1931	rVB5	1711168	3079742	32.88%	3.827%
21	14.533	1944	1948	1949	rBV4	1078529	1331796	14.22%	1.655%
22	14.569	1950	1954	1962	rVB2	4071671	8334917	88.97%	10.359%
23	15.356	2085	2088	2094	rBV	1694147	2081643	22.22%	2.587%
24	16.061	2206	2208	2212	rVB	2365187	2804138	29.93%	3.485%
25	16.302	2247	2249	2254	rVB	4321202	5306434	56.64%	6.595%
26	19.939	2865	2868	2877	rVB	6097992	9367955	100.00%	11.642%
27	21.584	3143	3148	3160	rVB2	4276059	7657949	81.75%	9.517%
28	24.751	3680	3687	3701	rVB	1851539	5635716	60.16%	7.004%

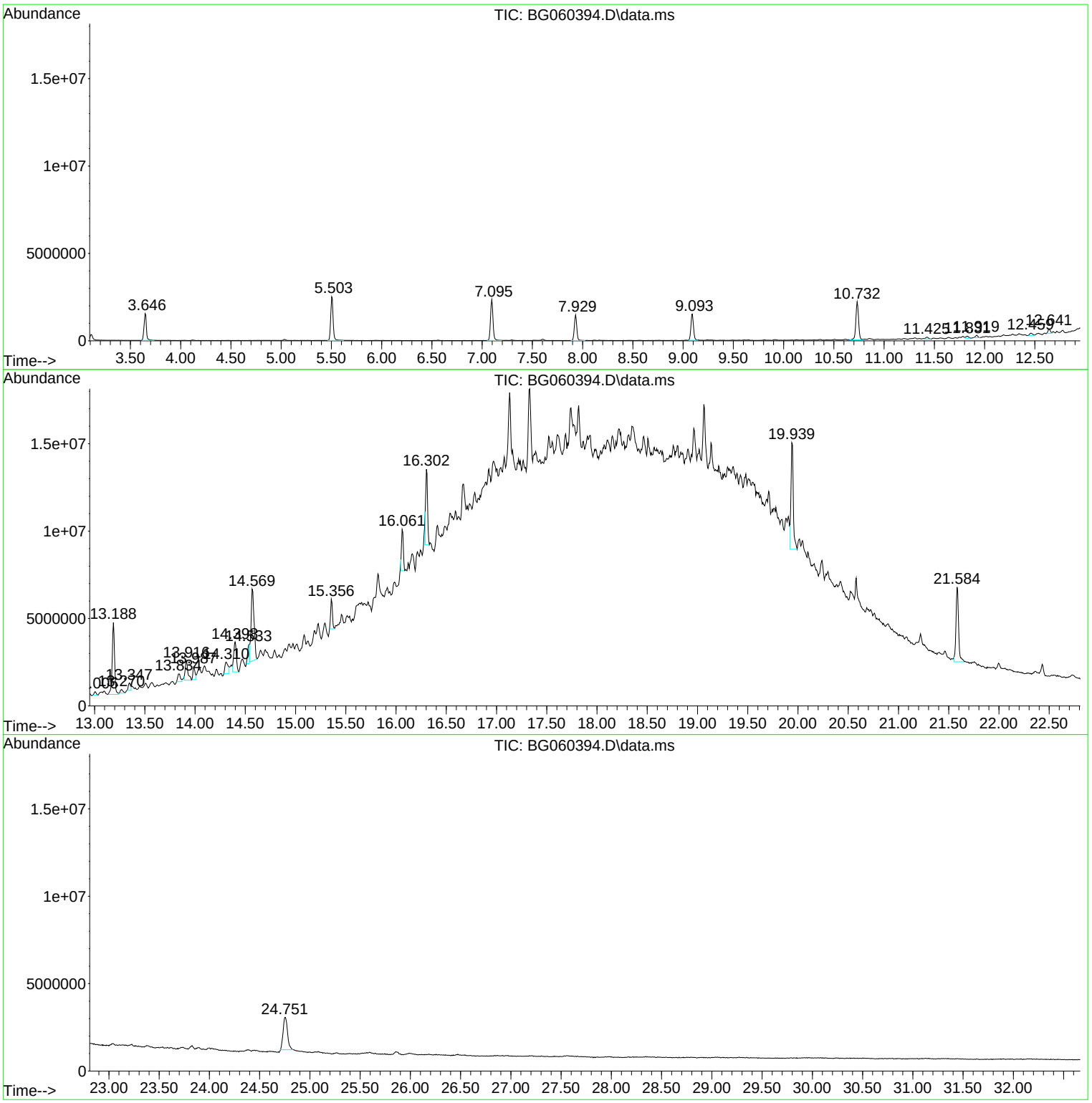
Sum of corrected areas: 80464239

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012224\
Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-24376

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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\BG012224\
Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

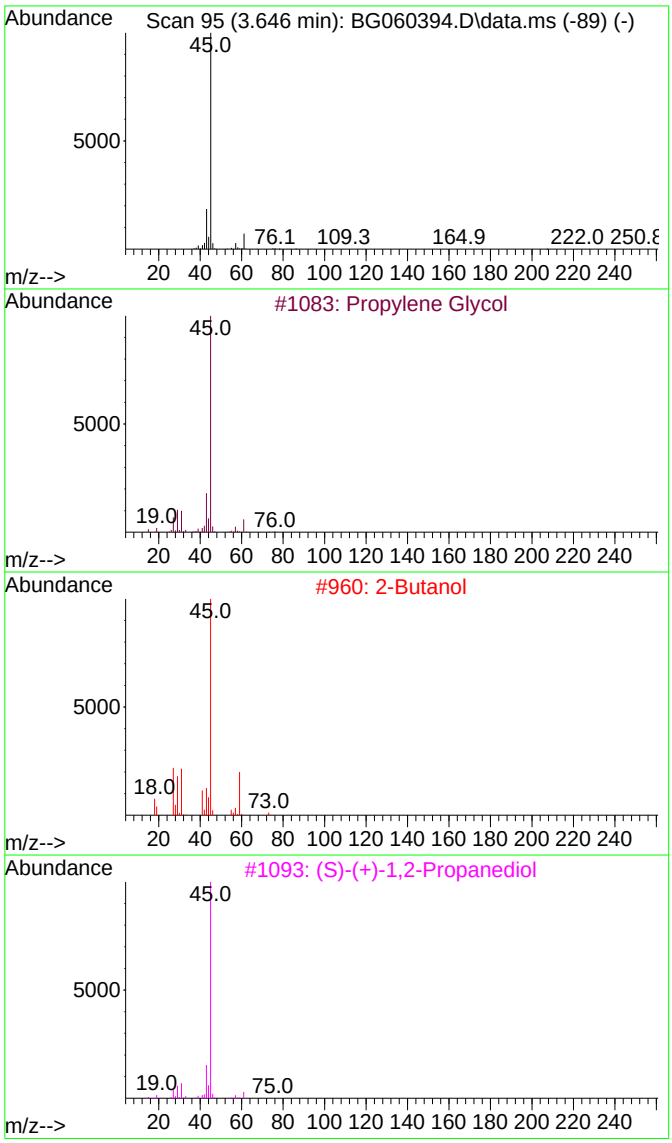
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

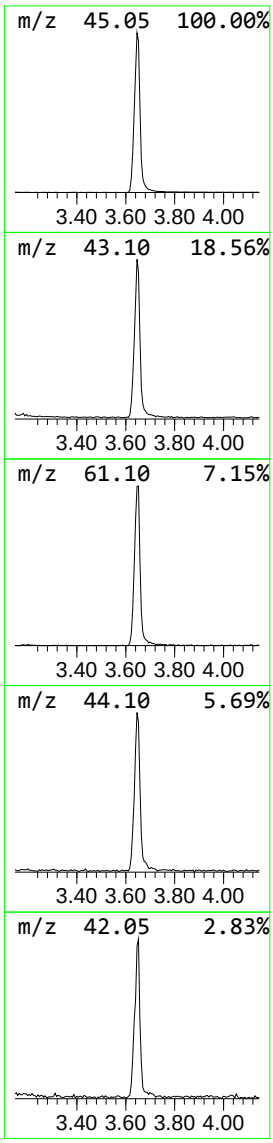
****

Peak Number 1 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.646	20.08 ng	2498970	1,4-Dichlorobenzene-d4	7.929

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	2-Butanol	74	C4H10O	000078-92-2	40
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012224\
Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-24376

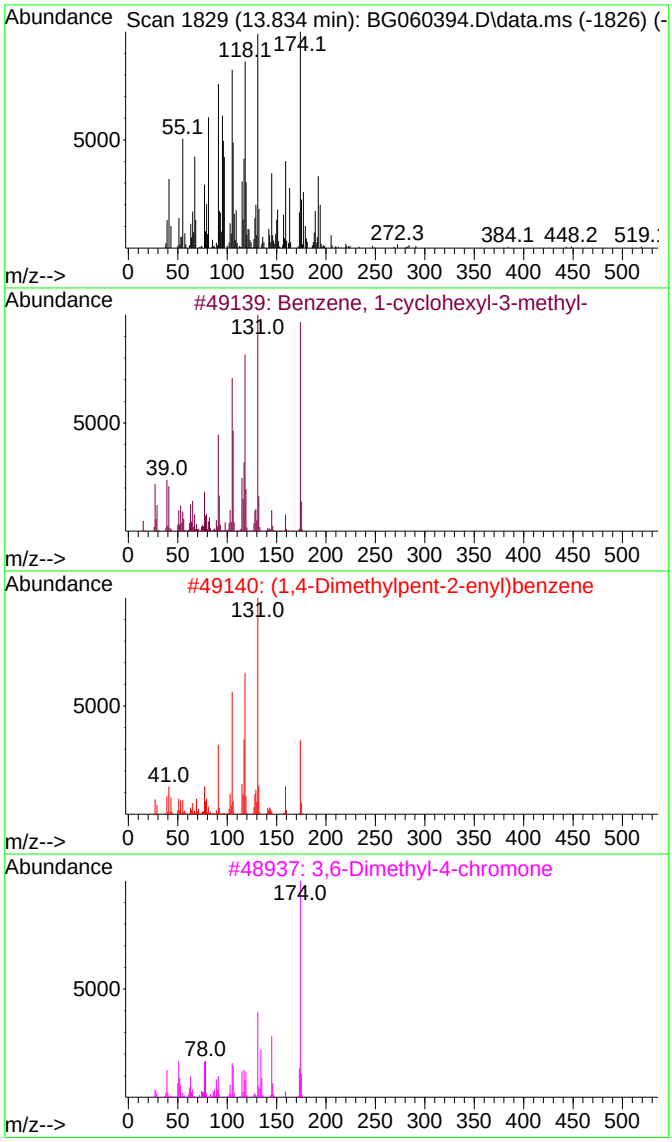
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

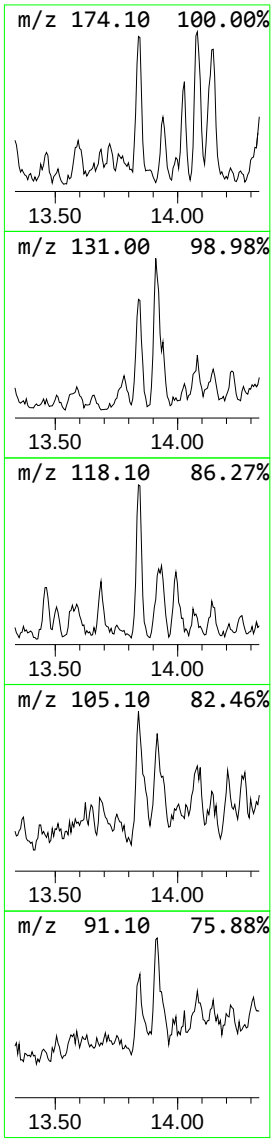
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-cyclohexyl-3-met... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.834	2.08 ng	867506	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	96
2	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	60
3	3,6-Dimethyl-4-chromone	174	C11H10O2	057646-01-2	55
4	1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	52
5	1H-1,3,2-Benzodiazaborole, 2-but...	174	C10H15BN2	031748-14-8	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012224\
Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
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Instrument :
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ClientSampleId :
CHRT-24376

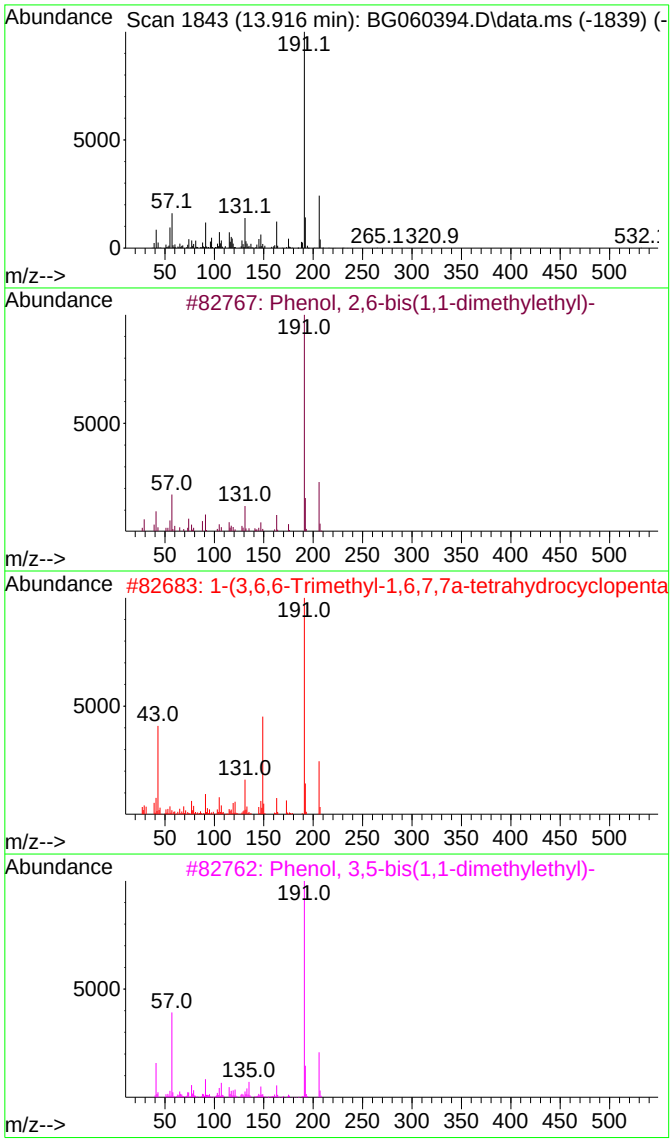
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

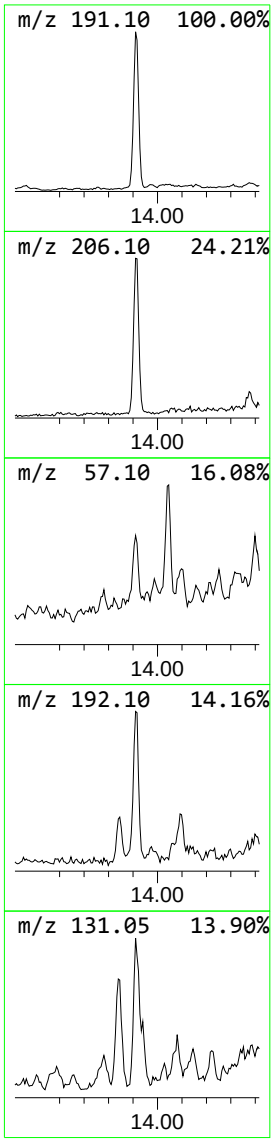
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	4.84 ng	2016280	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	95
2	1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	90
3	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	87
4	3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	87
5	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012224\
Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-24376

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

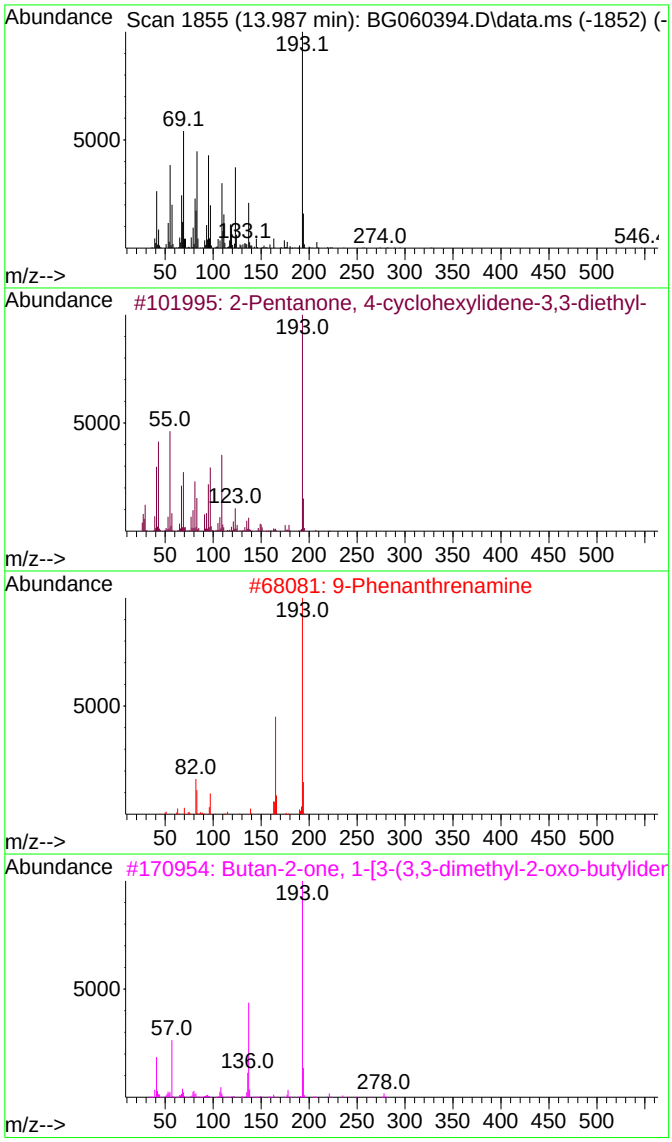
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

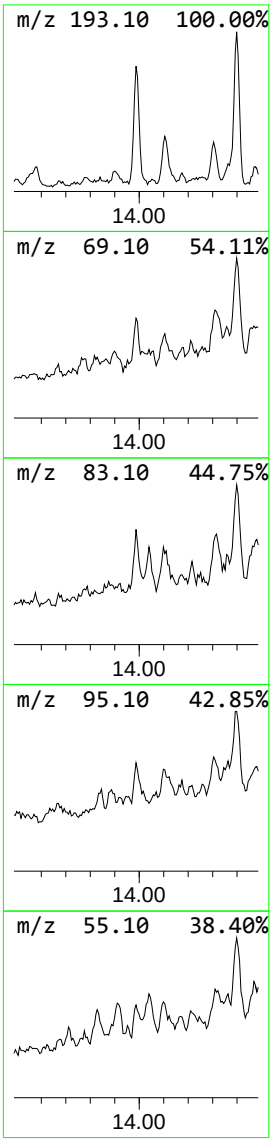
****

Peak Number 4 unknown13.987 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.987	2.60 ng	1083200	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	43
2	9-Phenanthrenamine	193	C14H11N	000947-73-9	27
3	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	27
4	3-Phenylindole	193	C14H11N	001504-16-1	25
5	Trisiloxane, 1,1,3,3,5,5-hexamet...	208	C6H20O2Si3	001189-93-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012224\
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Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-24376

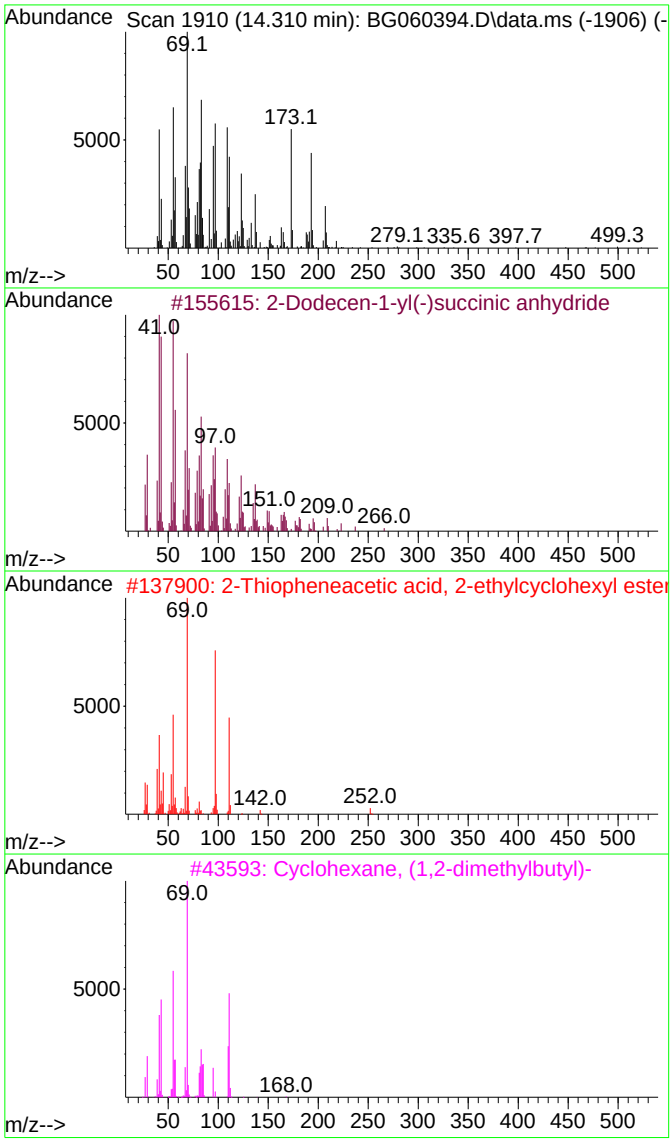
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

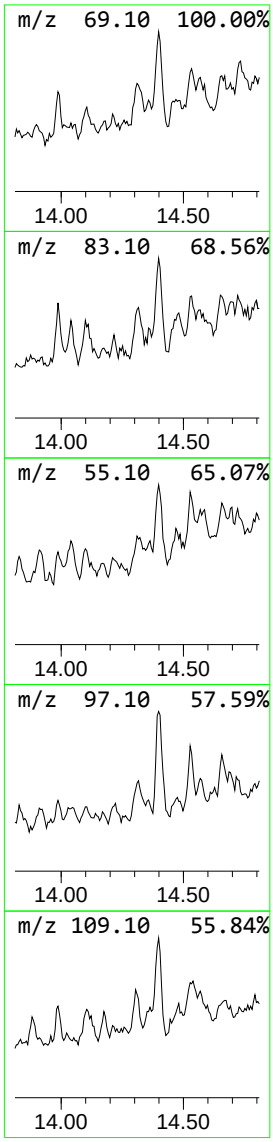
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Dodecen-1-yl(-)succinic a... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	3.57 ng	1489130	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	50
2	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	27
3	Cyclohexane, (1,2-dimethylbutyl)-	168	C12H24	061142-37-8	25
4	Oleyl alcohol, trifluoroacetate	364	C20H35F3O2	1000352-68-4	25
5	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012224\
Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-24376

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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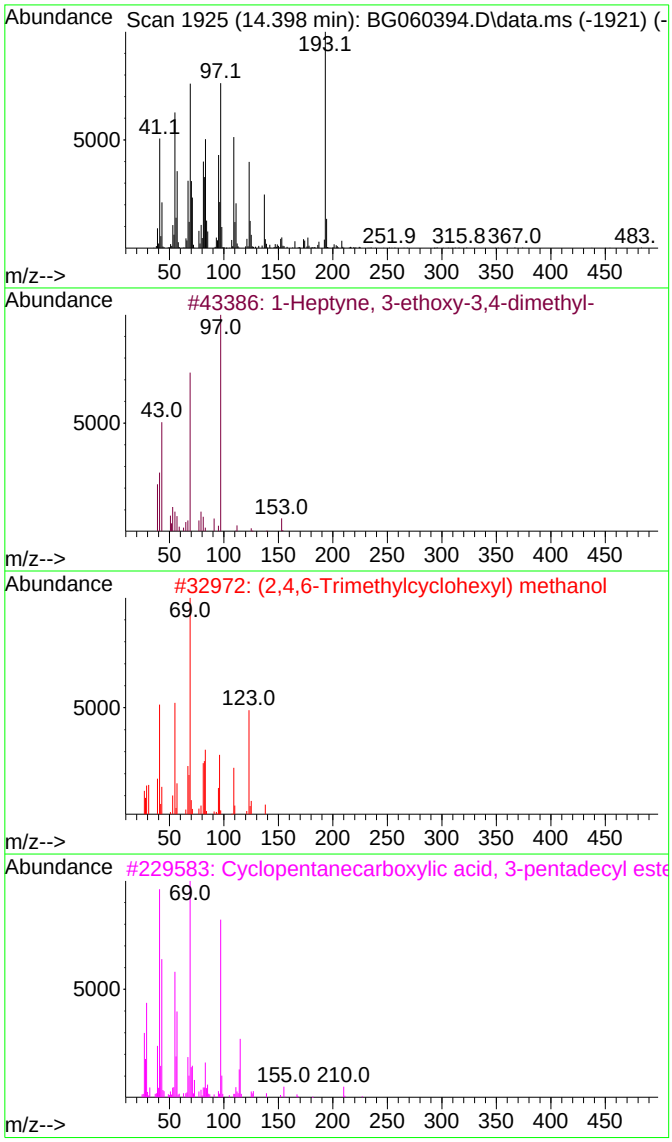
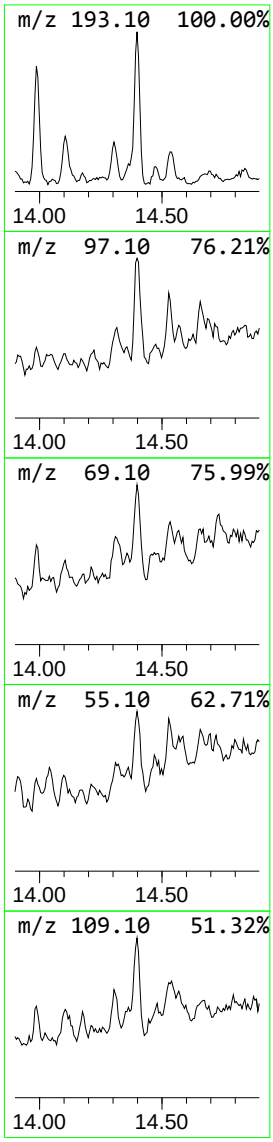
****

Peak Number 6 unknown14.398 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.398	7.39 ng	3079740	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptyne, 3-ethoxy-3,4-dimethyl-	168	C11H20O	054411-04-0	22
2	(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
3	Cyclopentanecarboxylic acid, 3-p...	324	C21H40O2	1000280-59-1	22
4	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	14
5	3-(But-3-enyl)-cyclohexanone	152	C10H16O	003636-03-1	11





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Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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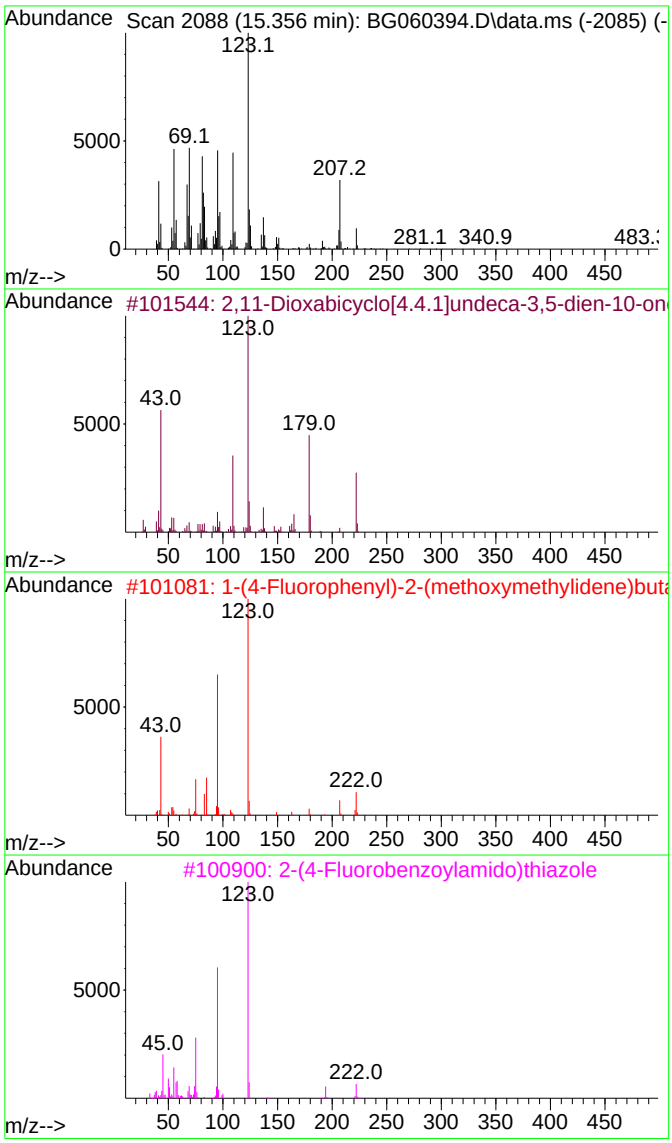
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

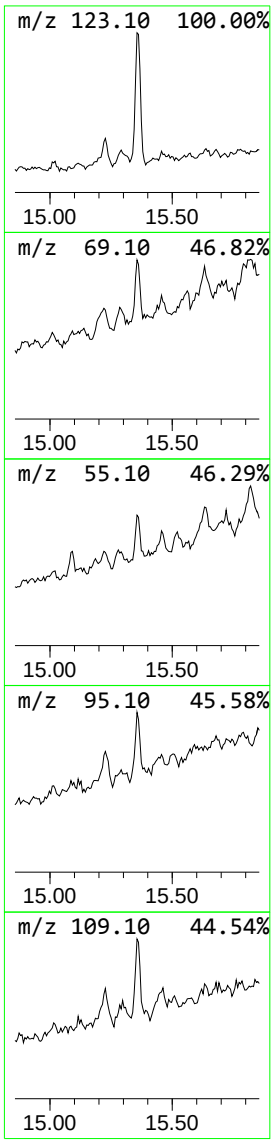
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.356	4.99 ng	2081640	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	50
2	1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	47
3	2-(4-Fluorobenzoylamido)thiazole	222	C10H7FN2OS	313376-92-0	43
4	4-Nitrophenyl bicyclo[4.1.0]hept...	261	C14H15NO4	328938-65-4	43
5	4-Fluoro-N-(1H-tetrazol-5-yl)ben...	207	C8H6FN5O	1000306-76-6	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

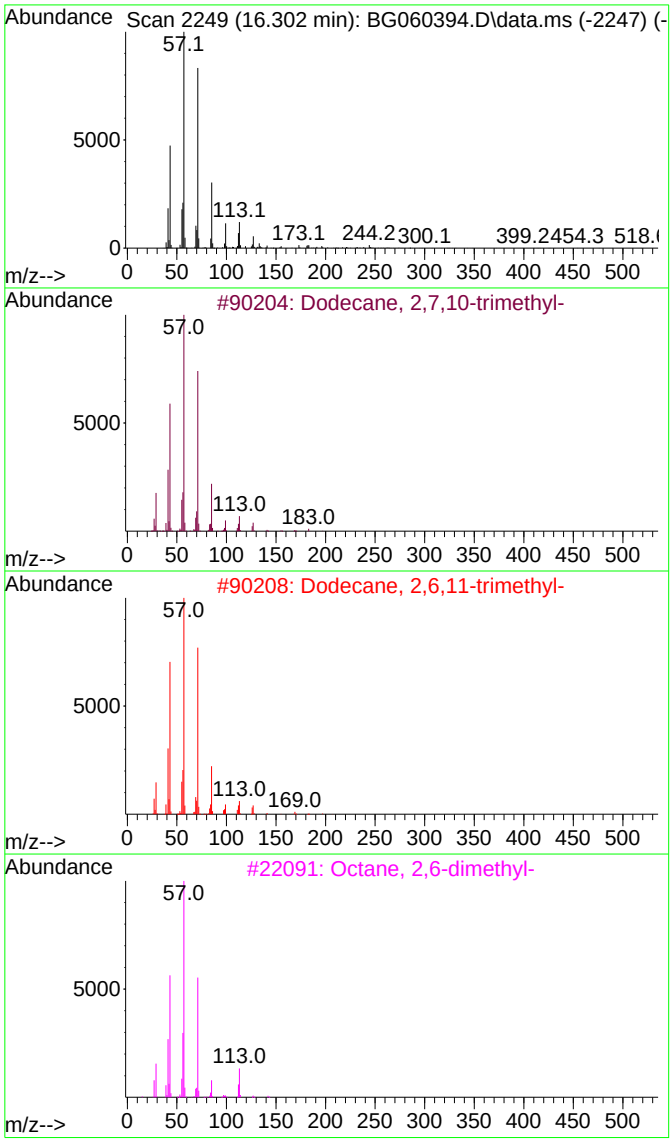
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

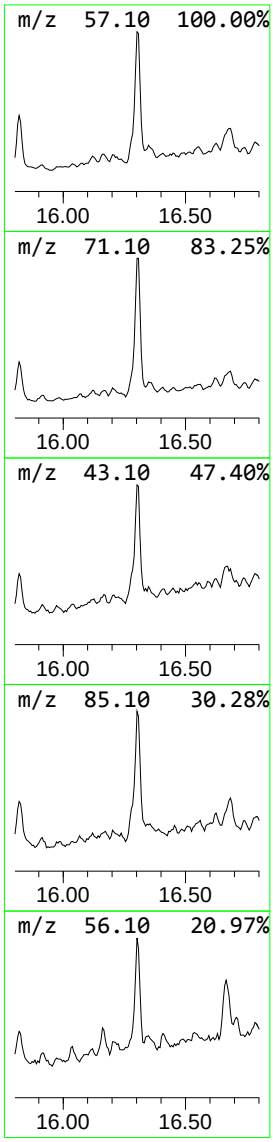
****

Peak Number 8 Dodecane, 2,7,10-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.302	20.00 ng	5306430	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	83
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
4	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
5	Heptacosane	380	C27H56	000593-49-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012224\
Data File : BG060394.D
Acq On : 22 Jan 2024 21:09
Operator : MA/JU
Sample : P1200-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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
Propylene Glycol	3.646	20.1	ng	2498970	1	7.929	2489280	20.0
Benzene, 1-cycl...	13.834	2.1	ng	867506	3	14.569	8334920	20.0
Phenol, 2,6-bis...	13.916	4.8	ng	2016280	3	14.569	8334920	20.0
unknown13.987	13.987	2.6	ng	1083200	3	14.569	8334920	20.0
2-Dodecen-1-yl(...	14.310	3.6	ng	1489130	3	14.569	8334920	20.0
unknown14.398	14.398	7.4	ng	3079740	3	14.569	8334920	20.0
2,11-Dioxabicyc...	15.356	5.0	ng	2081640	3	14.569	8334920	20.0
Dodecane, 2,7,1...	16.302	20.0	ng	5306430	4	17.330	5306430	20.0