LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060214.D
Acq On : 3 Jan 2024 5:18
Operator : MA/JU
Sample : 05899-20
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GHL-SS-07-2-4

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-BG122923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	10	rVB	361158	376590	3.03%	0.546%
2	5.044	327	333	337	rBV2	91810	140882	1.13%	0.204%
3	5.508	405	412	432	rBV	3145756	5384321	43.38%	7.806%
4	7.100	676	683	703	rBV	3210529	5599713	45.11%	8.119%
5	7.935	815	825	837	rBV	740995	1358048	10.94%	1.969%
6	9.098	1016	1023	1032	rBV	1838251	3307519	26.65%	4.795%
7	10.743	1292	1303	1309	rBV	1145615	2097843	16.90%	3.041%
8	10.784	1309	1310	1322	rVB2	85665	144131	1.16%	0.209%
9	12.400	1576	1585	1592	rVB	106660	194206	1.56%	0.282%
10	12.618	1616	1622	1628	rBV	101853	174715	1.41%	0.253%
11	13.199	1712	1721	1732	rBV	5641511	8914822	71.82%	12.925%
12	13.893	1834	1839	1844	rBV2	81606	145846	1.17%	0.211%
13	14.574	1943	1955	1963	rBV	2329686	3539704	28.52%	5.132%
14	14.968	2017	2022	2028	rBV	87963	143873	1.16%	0.209%
15	15.608	2127	2131	2136	rBV2	129022	199361	1.61%	0.289%
16	16.061	2200	2208	2219	rBV	4415500	6847702	55.17%	9.928%
17	16.301	2240	2249	2255	rBV	290728	513950	4.14%	0.745%
18	16.866	2339	2345	2353	rVB4	71433	139071	1.12%	0.202%
19	17.071	2371	2380	2384	rBV3	91988	144105	1.16%	0.209%
20	17.324	2416	2423	2428	rBV	2892104	4416663	35.58%	6.403%
21	17.365	2428	2430	2439	rVV	191745	281161	2.27%	0.408%
22	17.453	2439	2445	2452	rVB	404831	641892	5.17%	0.931%
23	17.723	2487	2491	2497	rVB	120923	174498	1.41%	0.253%
24	18.211	2569	2574	2579	rBV2	304876	482311	3.89%	0.699%
25	18.505	2620	2624	2628	rBV2	94670	129899	1.05%	0.188%
26	19.139	2724	2732	2738	rBV2	108574	186629	1.50%	0.271%
27	19.944	2862	2869	2881	rBV	9002707	12412707	100.00%	17.996%
28	21.237	3084	3089	3097	rBV	666445	1056802	8.51%	1.532%
29	21.589	3142	3149	3160	rBV2	2520944	4383216	35.31%	6.355%
30	22.383	3279	3284	3295	rVB7	104633	268017	2.16%	0.389%
31	23.851	3530	3534	3540	rVB5	77178	166691	1.34%	0.242%
32	24.762	3679	3689	3705	rVB	1615335	4572535	36.84%	6.629%
33	25.908	3877	3884	3894	rVB5	62058	201150	1.62%	0.292%
34	26.037	3897	3906	3911	rBV9	74931	233664	1.88%	0.339%

Sum of corrected areas: 68974237

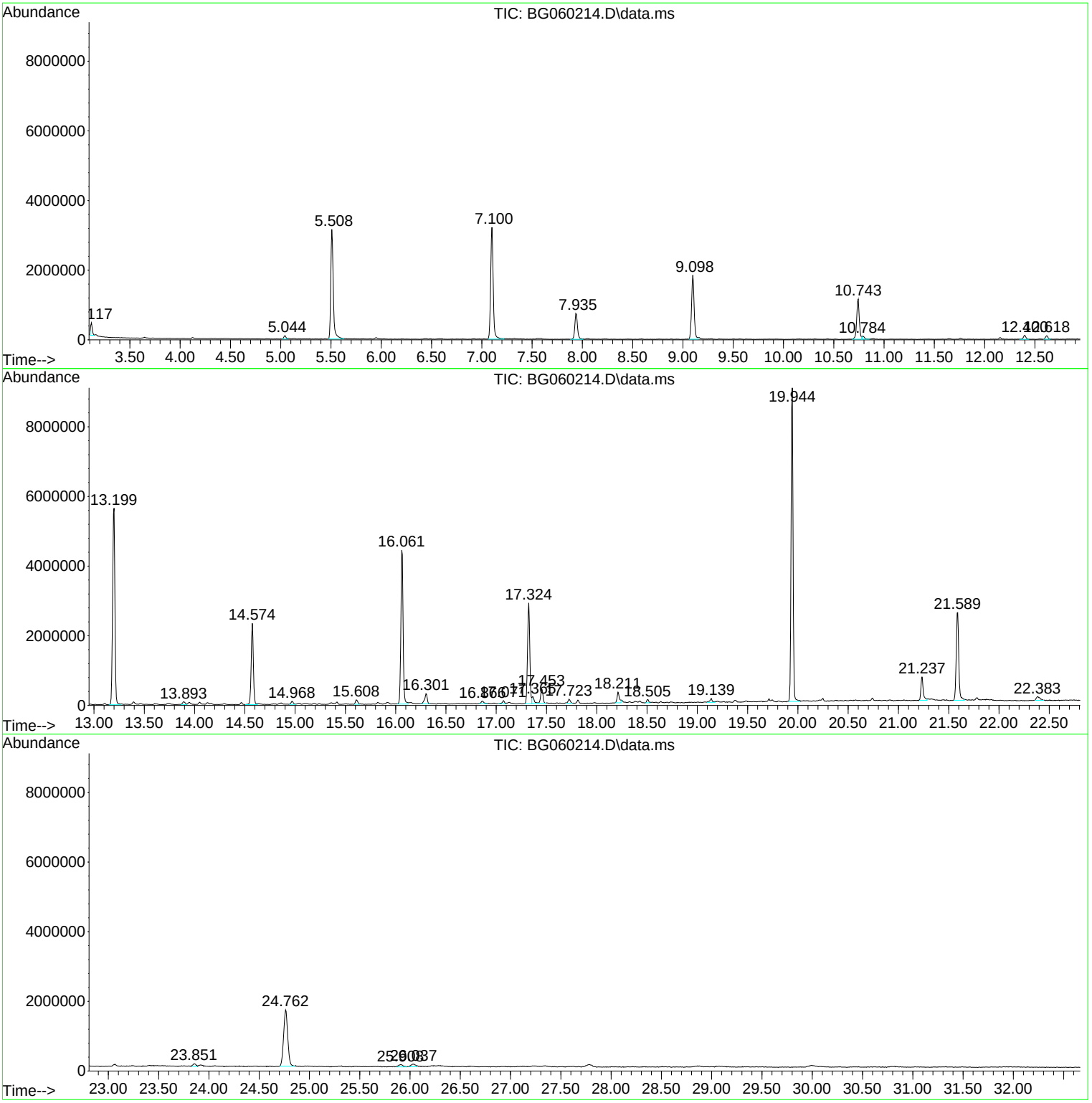
Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-2-4

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060214.D
Acq On : 3 Jan 2024 5:18
Operator : MA/JU
Sample : 05899-20
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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\BG010224\
Data File : BG060214.D
Acq On : 3 Jan 2024 5:18
Operator : MA/JU
Sample : 05899-20
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-2-4

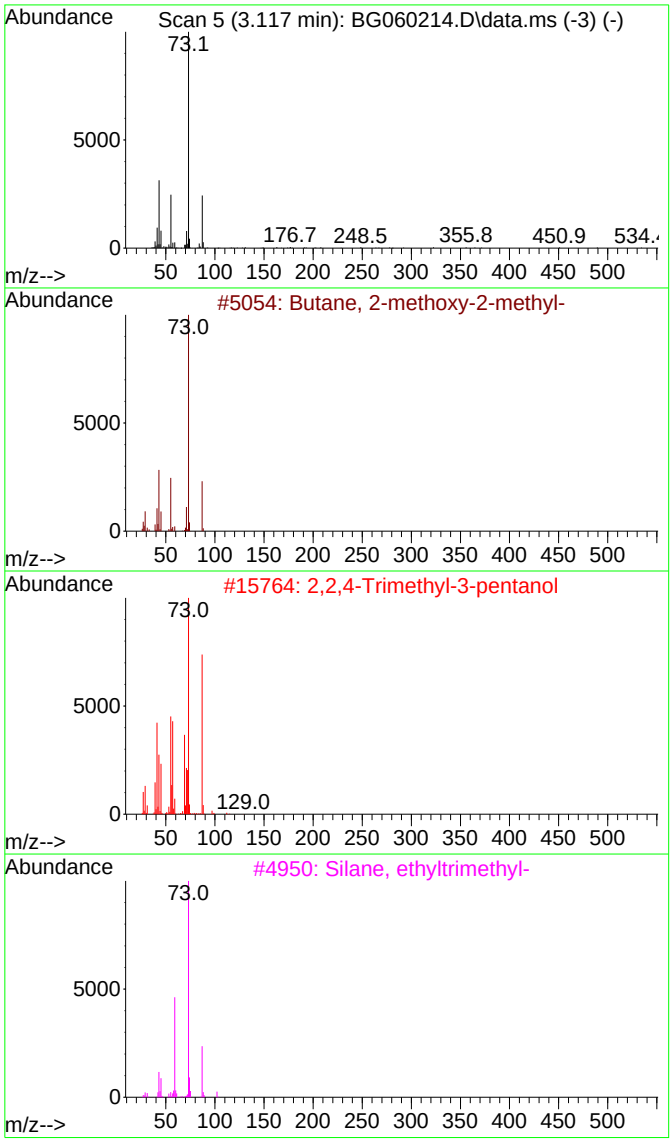
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

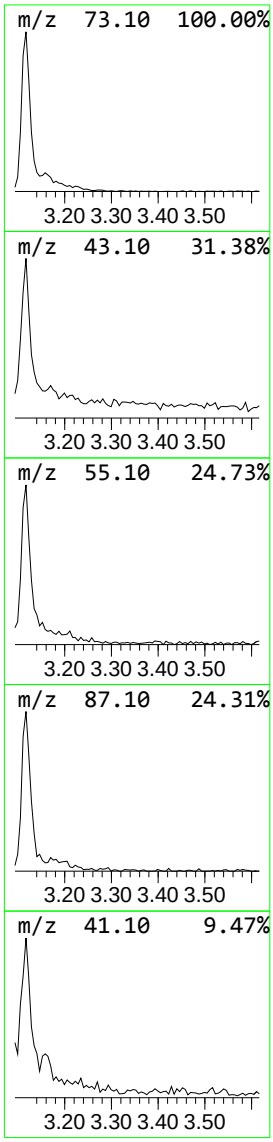
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	5.55 ng	376590	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060214.D
Acq On : 3 Jan 2024 5:18
Operator : MA/JU
Sample : 05899-20
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-2-4

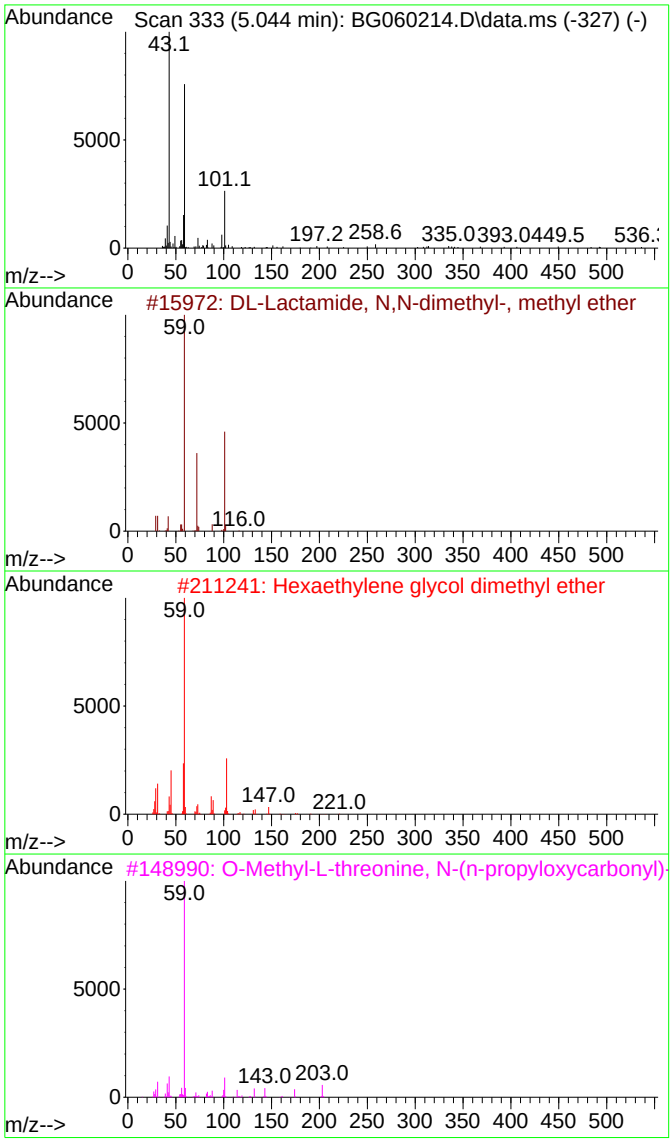
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

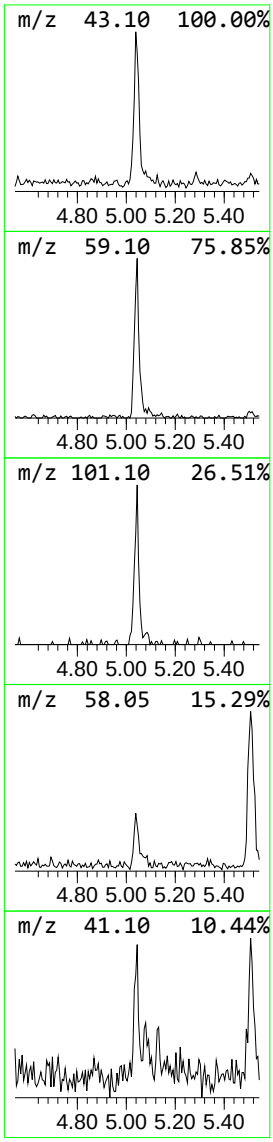
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 DL-Lactamide, N,N-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.044	2.07 ng	140882	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	50
2	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	38
3	O-Methyl-L-threonine, N-(n-propy...	261	C12H23NO5	1000453-24-8	33
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
5	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060214.D
Acq On : 3 Jan 2024 5:18
Operator : MA/JU
Sample : 05899-20
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-2-4

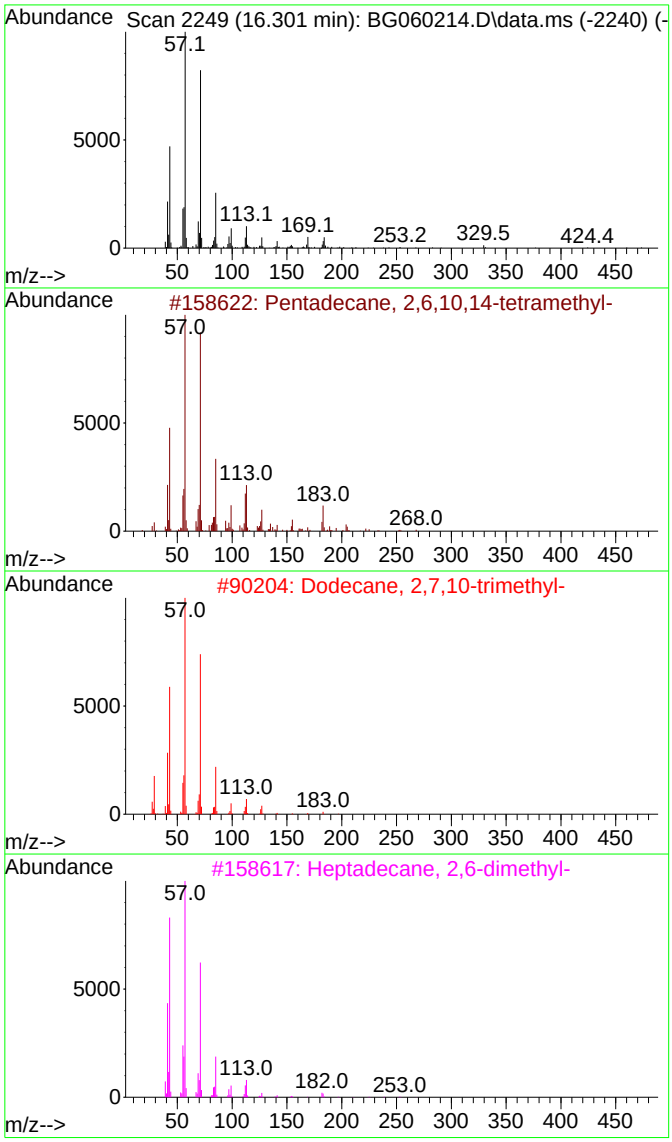
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

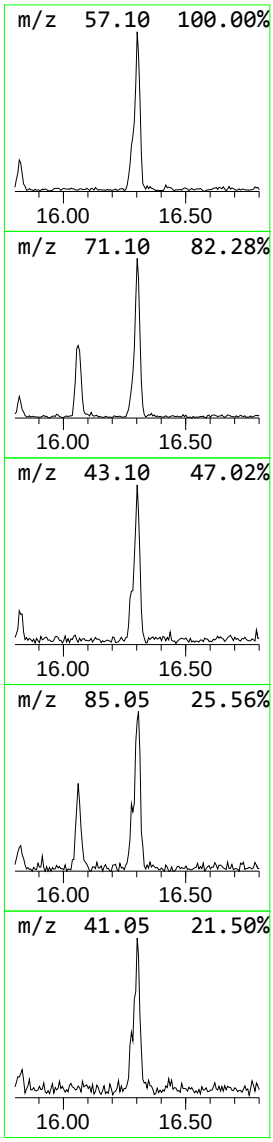
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentadecane, 2,6,10,14-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.301	2.33 ng	513950	Phenanthrene-d10	17.324

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	87
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
3	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	78
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
5	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060214.D
Acq On : 3 Jan 2024 5:18
Operator : MA/JU
Sample : 05899-20
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

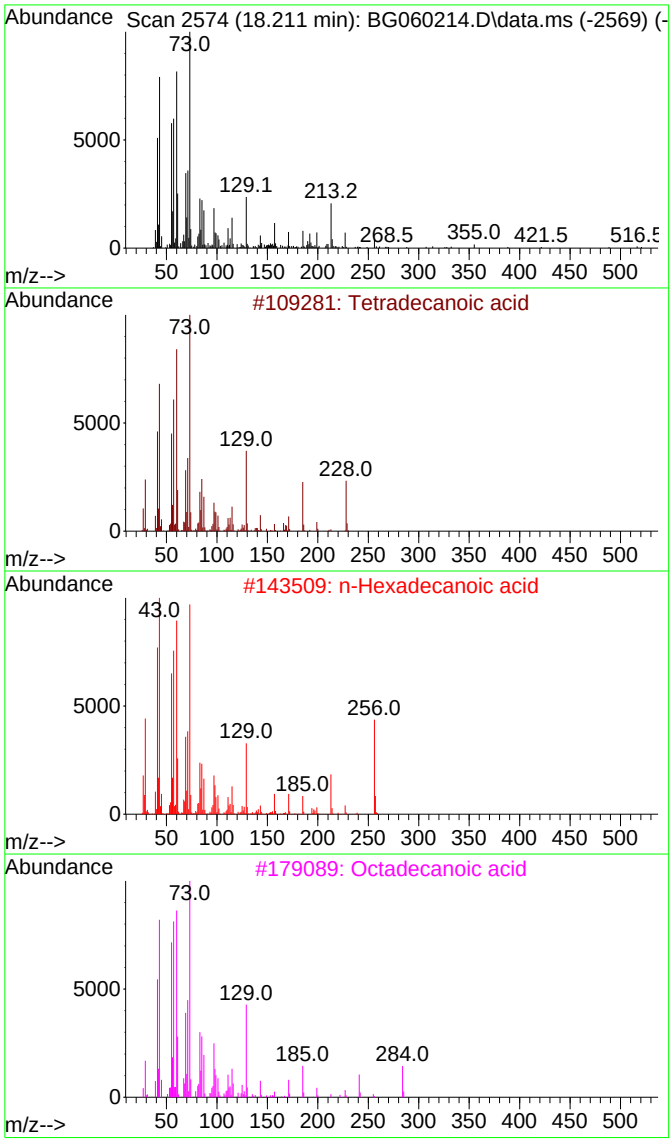
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

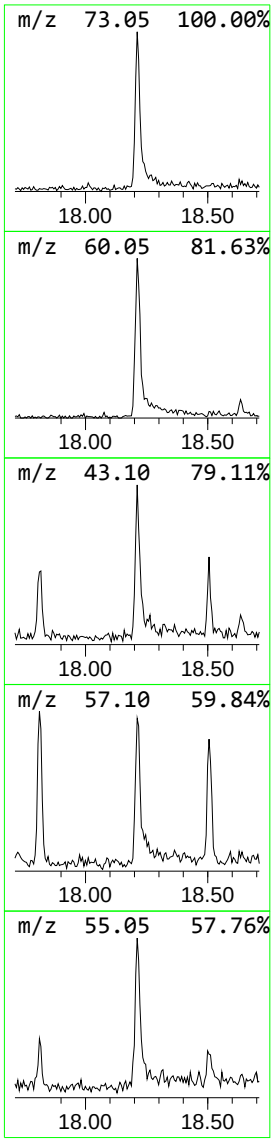
****

Peak Number 4 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	2.18 ng	482311	Phenanthrene-d10	17.324

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3	Octadecanoic acid	284	C18H36O2	000057-11-4	68
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060214.D
Acq On : 3 Jan 2024 5:18
Operator : MA/JU
Sample : 05899-20
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

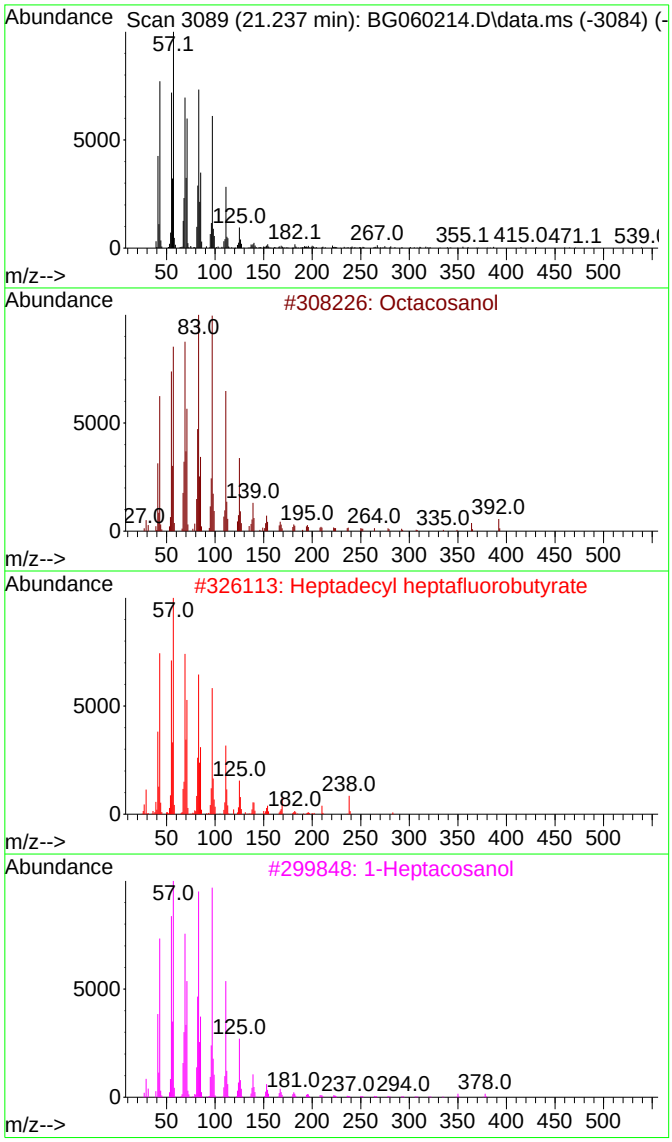
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

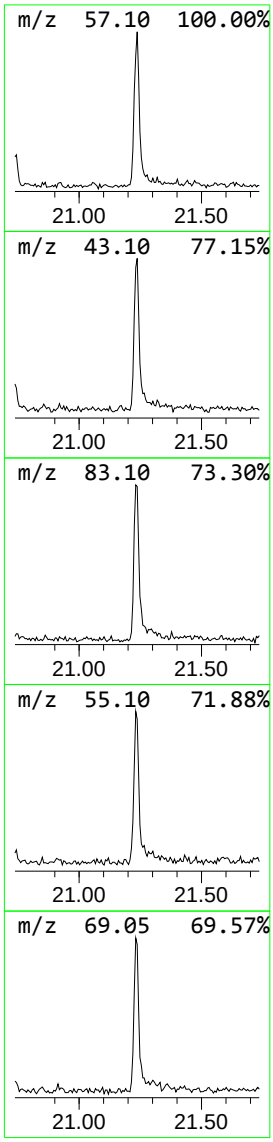
****

Peak Number 5 Octacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	4.82 ng	1056800	Chrysene-d12	21.589

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	87
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	86
5	Behenic alcohol	326	C22H46O	000661-19-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060214.D
Acq On : 3 Jan 2024 5:18
Operator : MA/JU
Sample : 05899-20
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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...	3.117	5.5	ng	376590	1	7.935	1358050	20.0
DL-Lactamide, N...	5.044	2.1	ng	140882	1	7.935	1358050	20.0
Pentadecane, 2,...	16.301	2.3	ng	513950	4	17.324	4416660	20.0
Tetradecanoic acid	18.211	2.2	ng	482311	4	17.324	4416660	20.0
Octacosanol	21.237	4.8	ng	1056800	5	21.589	4383220	20.0