LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG072418\
Data File : BG035841.D
Acq On : 24 Jul 2018 10:34
Operator : JU/SJ
Sample : PB111227BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId :

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-BG071218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.138	308	315	322	rBV	117649	185956	4.02%	0.884%
2	5.608	389	395	411	rBV	851731	1458119	31.54%	6.935%
3	7.200	658	666	676	rBV	880017	1578285	34.14%	7.507%
4	7.564	720	728	737	rBV	858503	1516318	32.80%	7.212%
5	8.028	798	807	817	rBV	164183	289441	6.26%	1.377%
6	8.345	854	861	872	rBV	636899	1142971	24.72%	5.436%
7	9.191	996	1005	1018	rBV	485252	942644	20.39%	4.483%
8	10.830	1276	1284	1304	rBV2	183826	374906	8.11%	1.783%
9	13.274	1692	1700	1710	rBV	1527540	2355935	50.96%	11.205%
10	14.648	1928	1934	1945	rBV2	328719	563412	12.19%	2.680%
11	16.141	2181	2188	2206	rBV	1278450	2089841	45.20%	9.940%
12	17.392	2390	2401	2413	rBV2	509957	837876	18.12%	3.985%
13	19.689	2786	2792	2800	rVB	252326	288006	6.23%	1.370%
14	19.800	2808	2811	2816	rVB	49581	57731	1.25%	0.275%
15	20.000	2838	2845	2854	rBV	3464846	4623525	100.00%	21.991%
16	20.728	2964	2969	2975	rVB	190472	214477	4.64%	1.020%
17	21.657	3120	3127	3137	rBV2	636383	1078881	23.33%	5.131%
18	21.839	3152	3158	3163	rBV2	39992	60247	1.30%	0.287%
19	22.438	3256	3260	3264	rBV4	33095	48056	1.04%	0.229%
20	23.125	3371	3377	3383	rBV2	39720	73397	1.59%	0.349%
21	23.918	3506	3512	3518	rVB3	38046	77331	1.67%	0.368%
22	24.852	3660	3671	3687	rBV2	342621	1029561	22.27%	4.897%
23	25.968	3853	3861	3869	rBV8	26378	71077	1.54%	0.338%
24	27.302	4080	4088	4099	rVB10	19754	66905	1.45%	0.318%

Sum of corrected areas: 21024898

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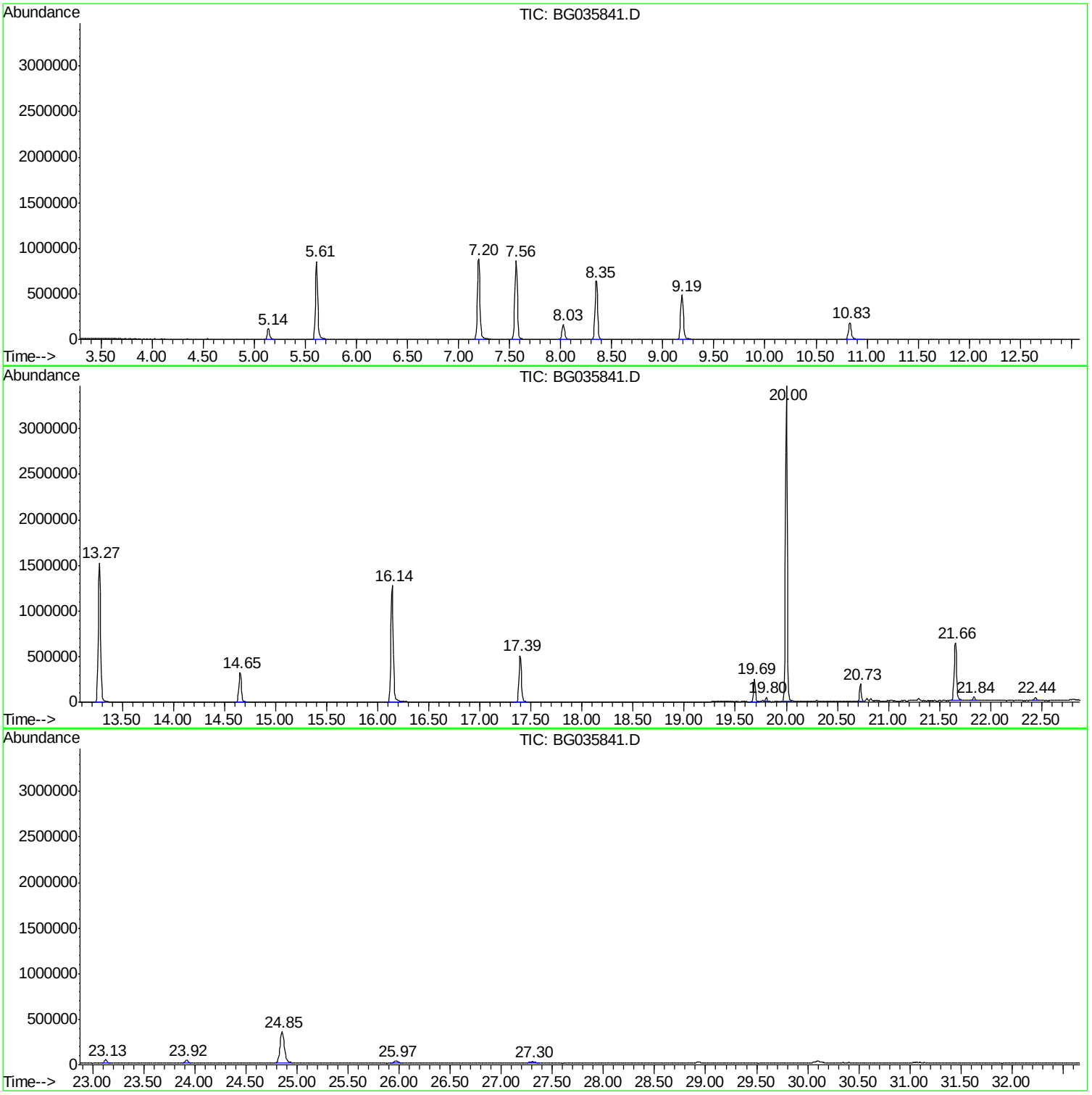
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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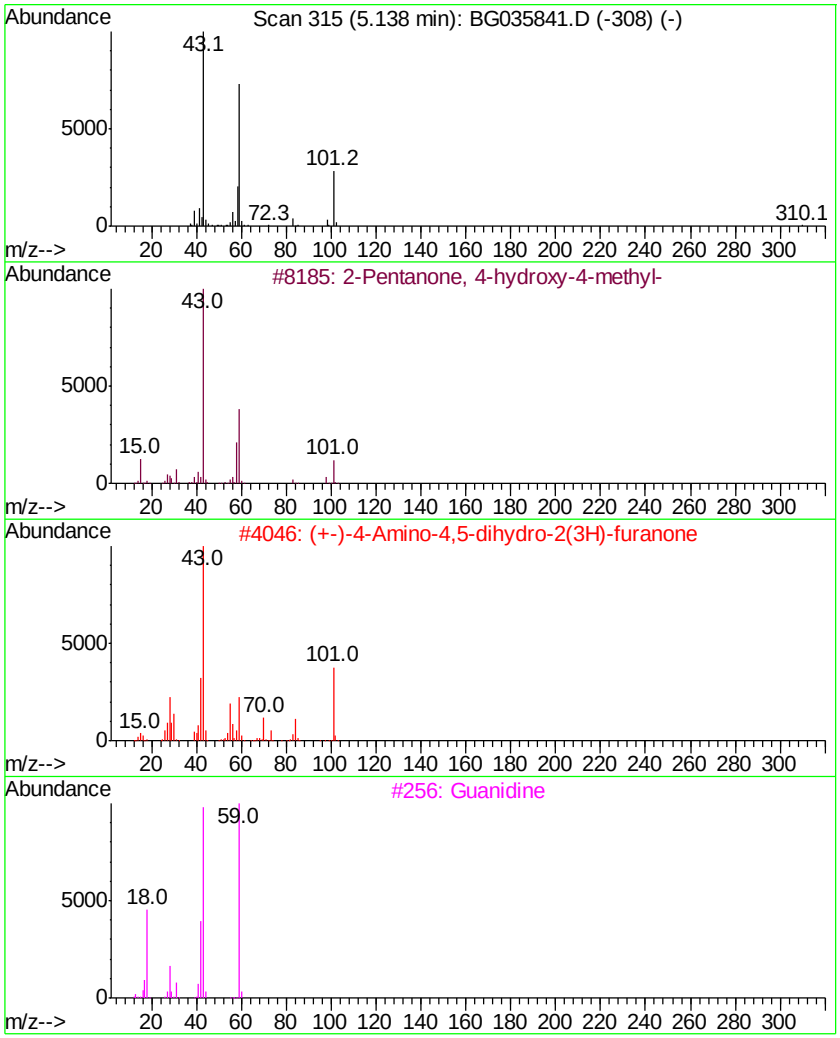
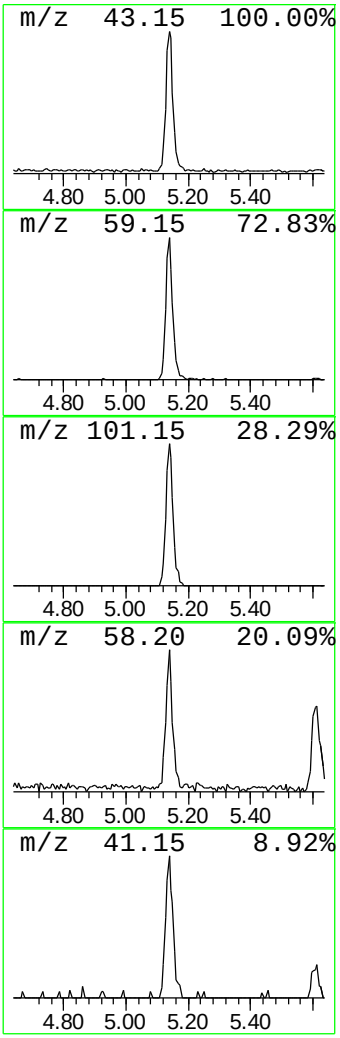
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	12.85 ng	185956	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Guanidine	59	CH5N3	000113-00-8	38
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG072418\
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Instrument : BNA_G
ClientSampleId :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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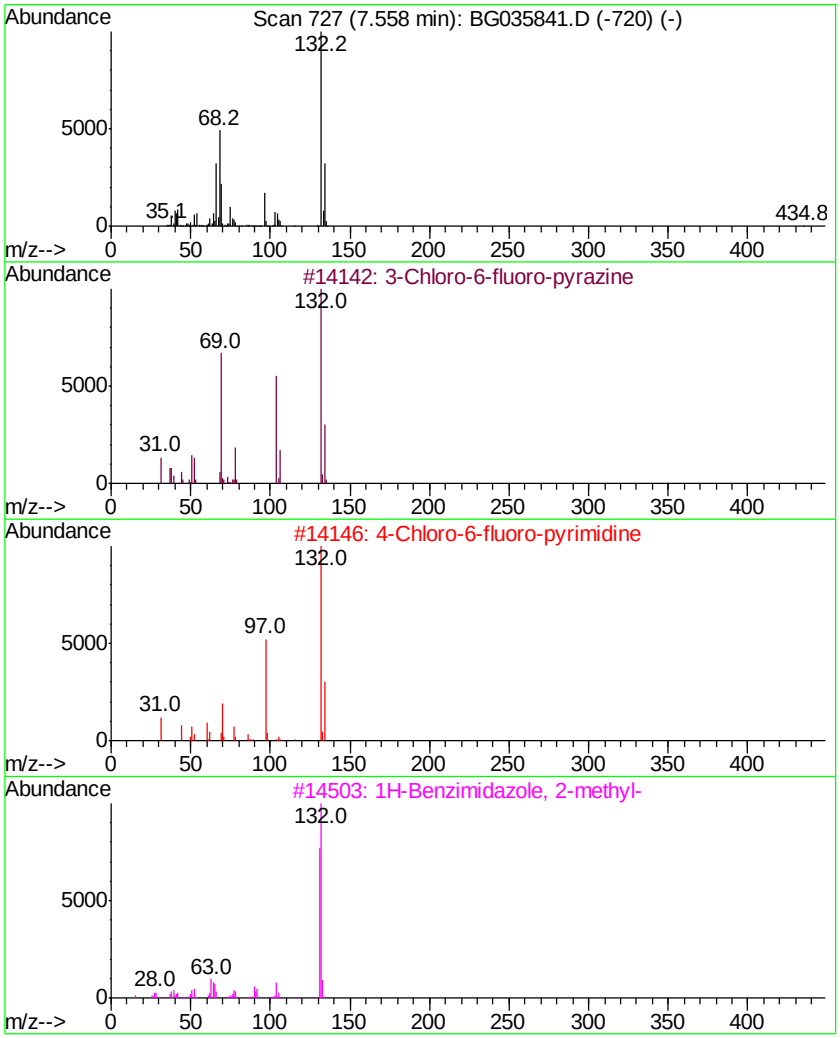
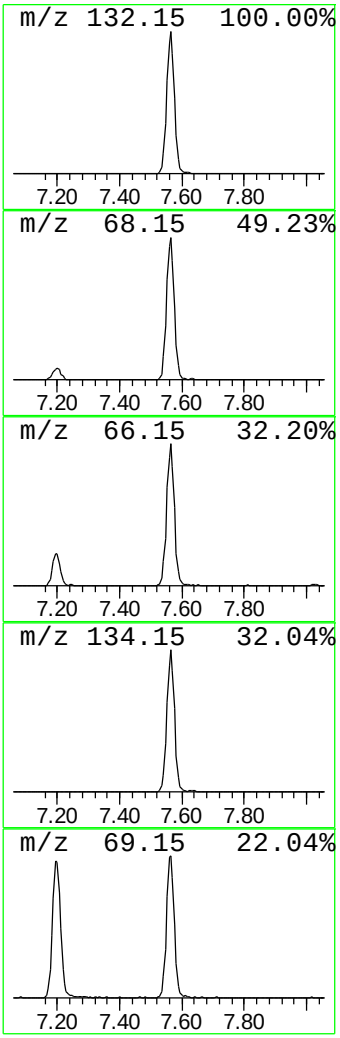
Peak Number 2 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	104.78 ng	1516320	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
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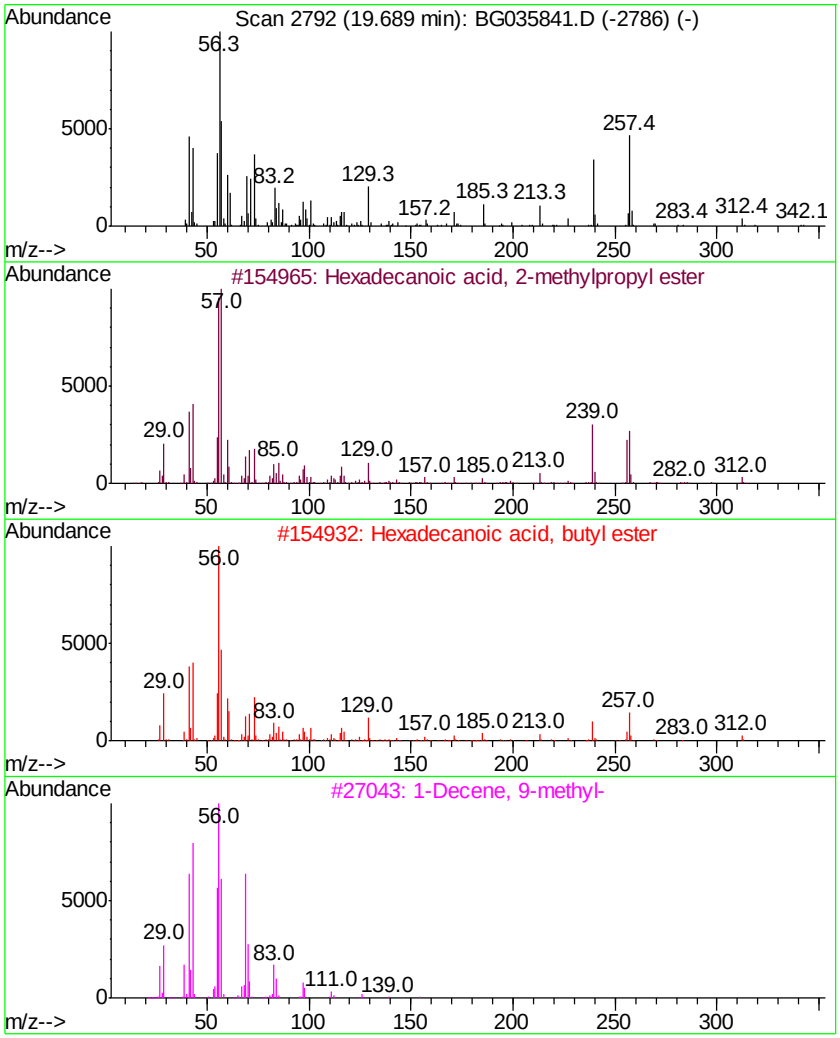
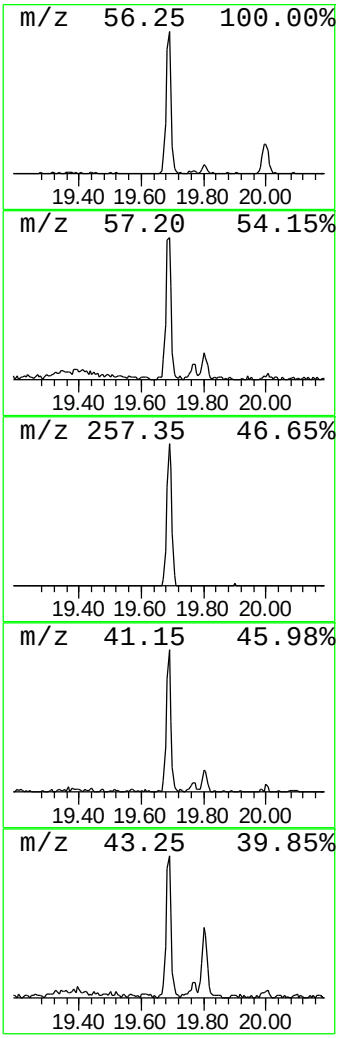
Peak Number 4 Hexadecanoic acid, 2-methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	5.34 ng	288006	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	93
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	92
3	1-Decene, 9-methyl-	154	C11H22	061142-78-7	25
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	22
5	5-Methyl-2-hexanol, trifluoroace...	212	C9H15F3O2	1000364-20-2	22





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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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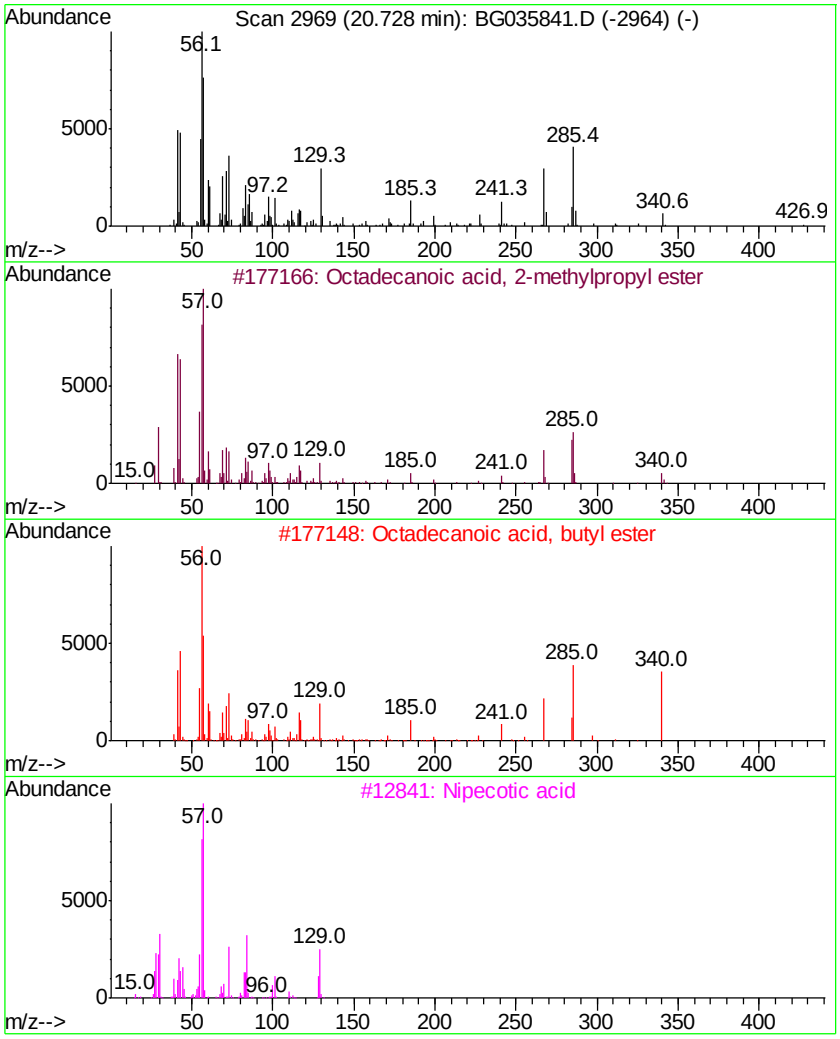
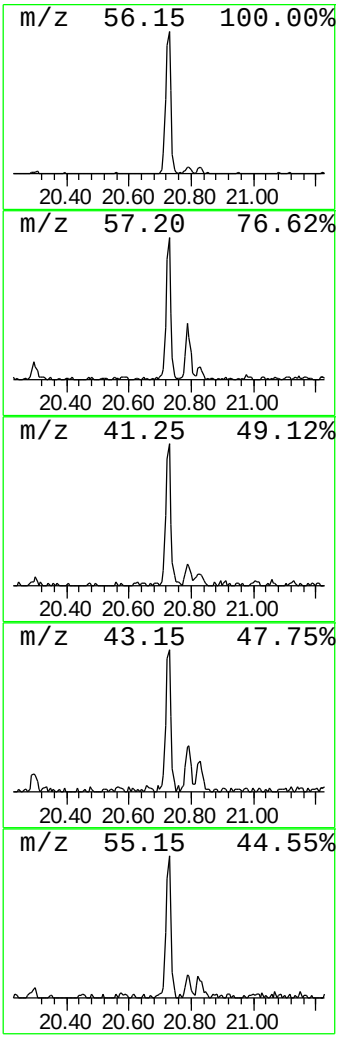
Peak Number 5 Octadecanoic acid, 2-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.73	3.98 ng	214477	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	90
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	86
3	Nipecotic acid	129	C6H11NO2	000498-95-3	32
4	2-Methylhexadec-1-ene	238	C17H34	061868-19-7	14
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	14





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	12.9	ng	185956	1	8.02	289441	20.0
unknown7.56	7.56	104.8	ng	1516320	1	8.02	289441	20.0
Hexadecanoic acid...	19.69	5.3	ng	288006	5	21.66	1078880	20.0
Octadecanoic acid...	20.73	4.0	ng	214477	5	21.66	1078880	20.0