LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102218\
Data File : BM017277.D
Acq On : 22 Oct 2018 13:53
Operator : MJ/SJ
Sample : J5575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SSSI-1015-S-DH-24-B

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_M\METHODS\8270-BM101718.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	4.834	308	314	324	rVB	200059	277023	2.08%	0.302%
2	5.275	383	389	398	rBV	4669300	6644130	49.80%	7.249%
3	6.846	648	656	671	rBV	4771358	7791964	58.40%	8.501%
4	7.199	707	716	728	rBV	4894621	7521735	56.38%	8.206%
5	7.663	787	795	803	rBV	1188236	1949045	14.61%	2.126%
6	7.975	841	848	856	rVB	3520654	5577749	41.80%	6.085%
7	8.816	983	991	1003	rBV	2860832	4638385	34.76%	5.061%
8	10.434	1257	1266	1281	rBV	1698693	2832458	21.23%	3.090%
9	12.916	1681	1688	1696	rBV	7119433	10772721	80.74%	11.753%
10	13.763	1826	1832	1842	rBV	596272	875991	6.57%	0.956%
11	14.304	1916	1924	1935	rBV2	2395216	3729976	27.96%	4.069%
12	15.798	2171	2178	2197	rBV	5649824	7992159	59.90%	8.720%
13	17.051	2384	2391	2404	rBV2	2927582	4311160	32.31%	4.704%
14	17.957	2540	2545	2554	rBV	372475	535933	4.02%	0.585%
15	19.245	2760	2764	2768	rBV2	111328	140268	1.05%	0.153%
16	19.692	2834	2840	2850	rBV	10652674	13342313	100.00%	14.557%
17	20.392	2954	2959	2962	rBV	339778	491464	3.68%	0.536%
18	20.439	2965	2967	2974	rVV2	169570	241998	1.81%	0.264%
19	20.504	2974	2978	2982	rVV2	157940	218294	1.64%	0.238%
20	20.974	3054	3058	3069	rBV	414134	672923	5.04%	0.734%
21	21.245	3099	3104	3113	rBV	3866257	4726266	35.42%	5.156%
22	21.356	3120	3123	3127	rBV4	86365	135487	1.02%	0.148%
23	21.409	3129	3132	3136	rVB	223842	232931	1.75%	0.254%
24	21.839	3202	3205	3208	rBV	266841	281831	2.11%	0.307%
25	22.098	3245	3249	3253	rBV	244689	317053	2.38%	0.346%
26	22.298	3279	3283	3290	rBV	294696	388907	2.91%	0.424%
27	22.421	3301	3304	3310	rVB	168568	227378	1.70%	0.248%
28	22.797	3364	3368	3373	rVB	311348	422627	3.17%	0.461%
29	23.350	3459	3462	3468	rVB2	262634	387909	2.91%	0.423%
30	23.456	3474	3480	3489	rVB	2137761	3980114	29.83%	4.342%

Sum of corrected areas: 91658192

LSC Report - Integrated Chromatogram

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102218\
Data File : BM017277.D
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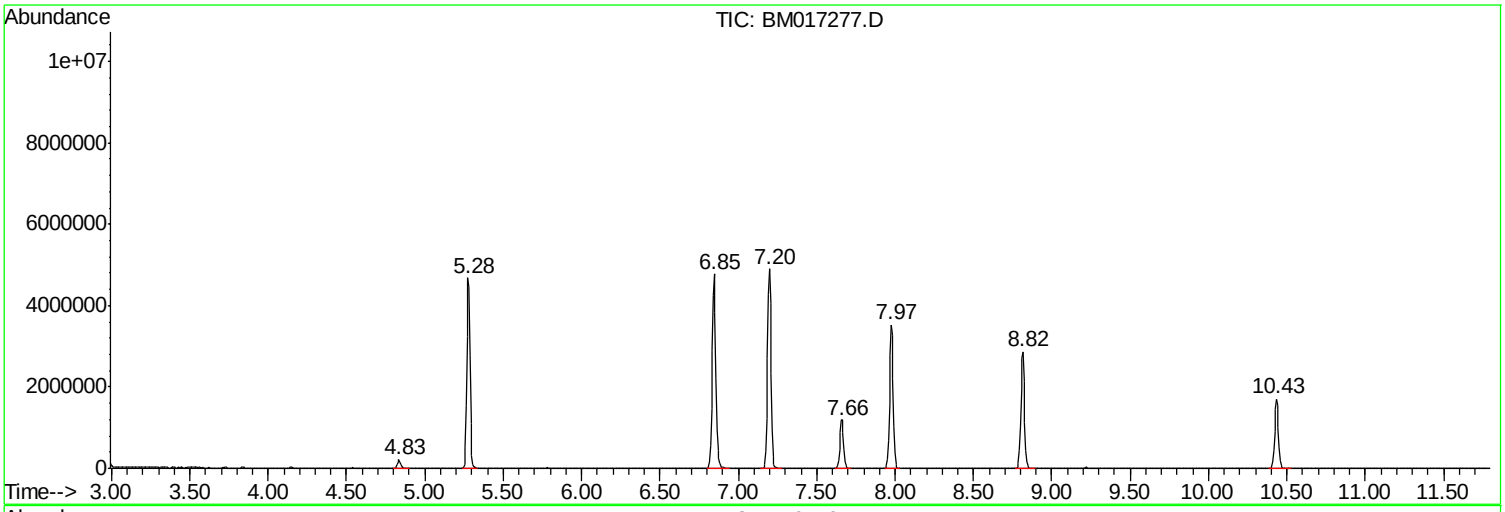
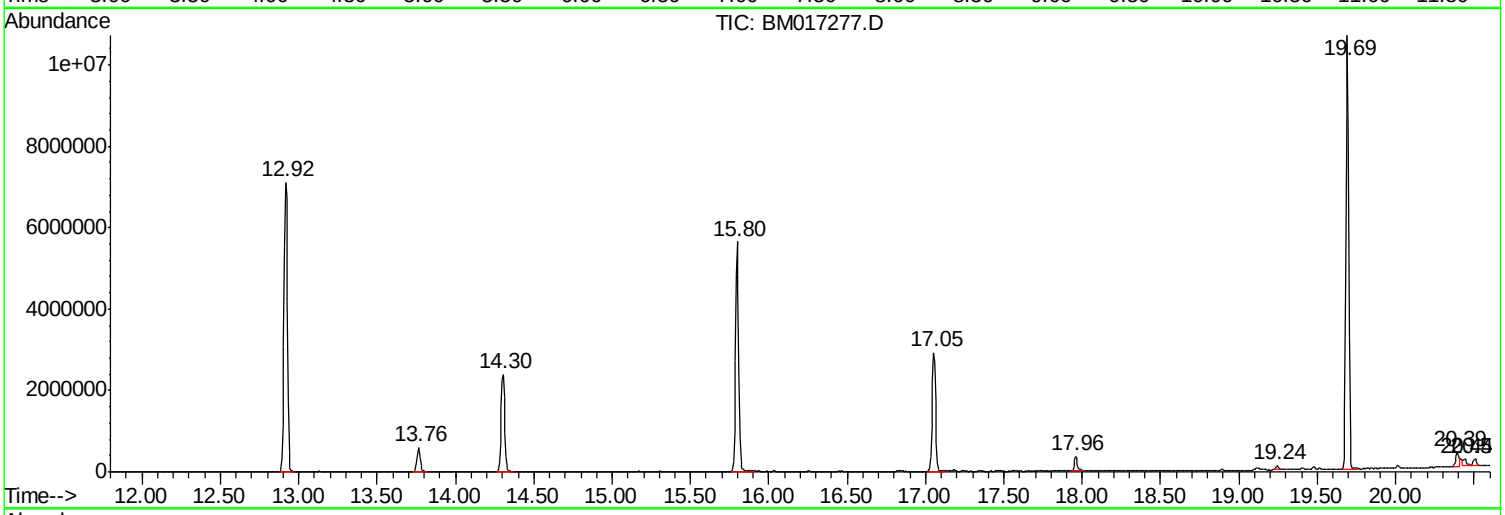
Operator : MJ/SJ
Sample : J5575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

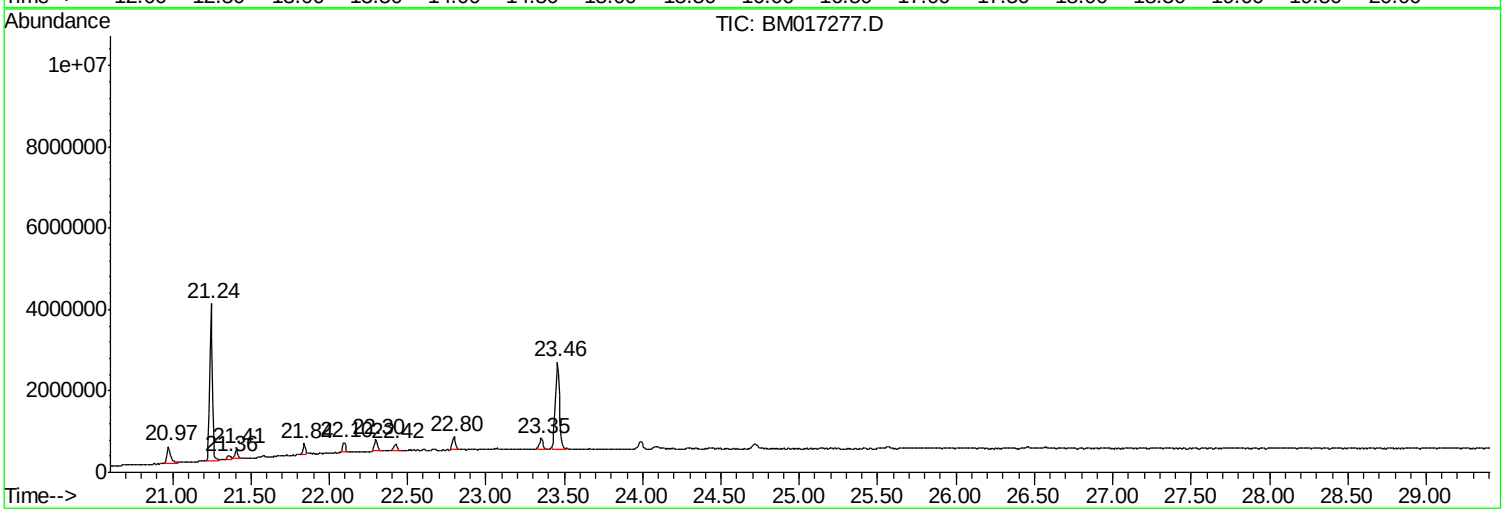
Instrument :
BNA_M
ClientSampleId :
SSSI-1015-S-DH-24-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P







Library Search Compound Report

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Data File : BM017277.D
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Instrument :
BNA_M
ClientSampleId :
SSSI-1015-S-DH-24-B

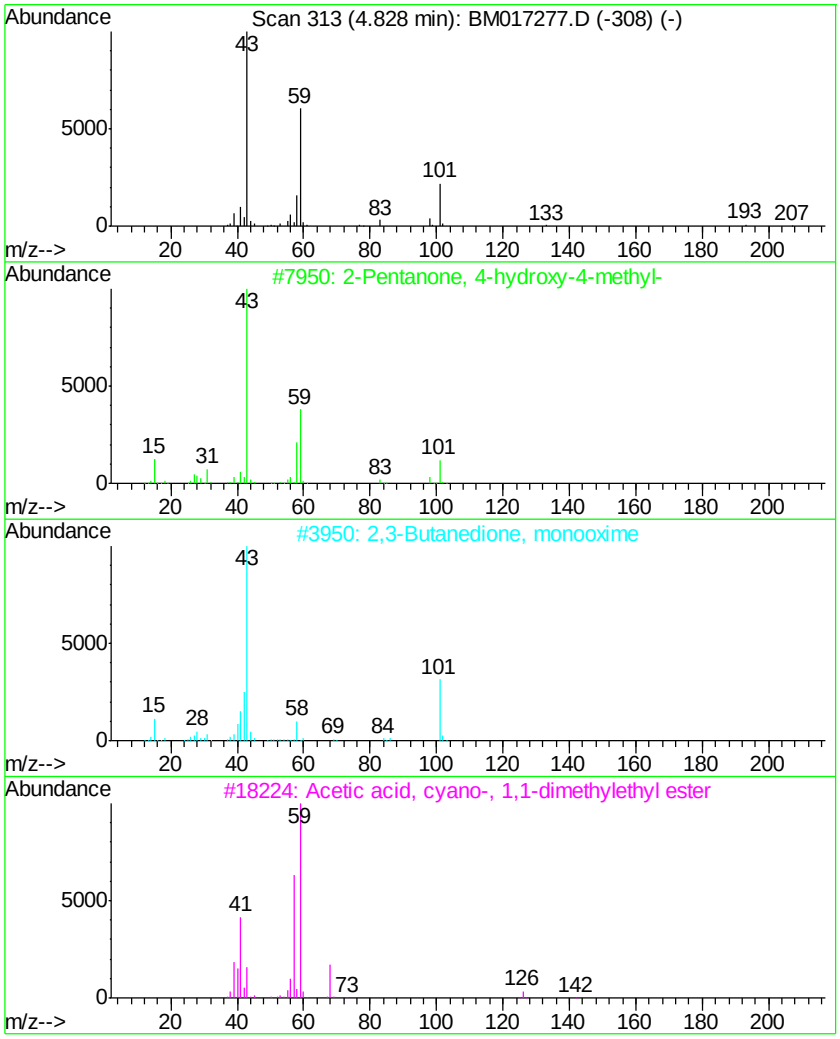
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

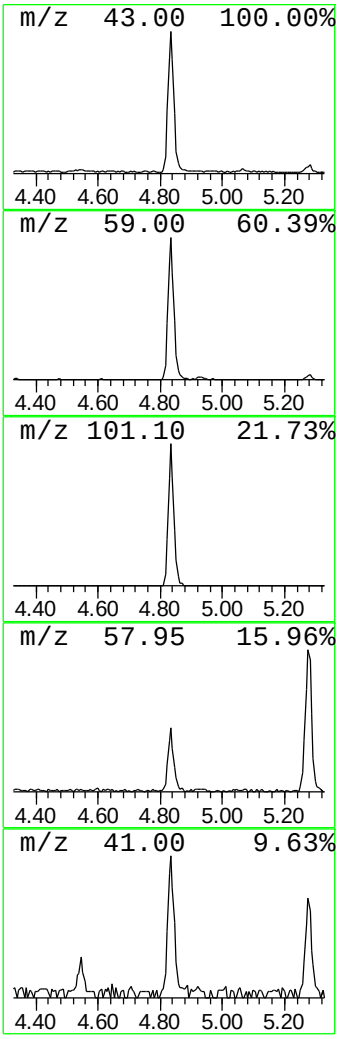
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	2.84 ng	277023	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102218\
Data File : BM017277.D
Acq On : 22 Oct 2018 13:53
Operator : MJ/SJ
Sample : J5575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SSSI-1015-S-DH-24-B

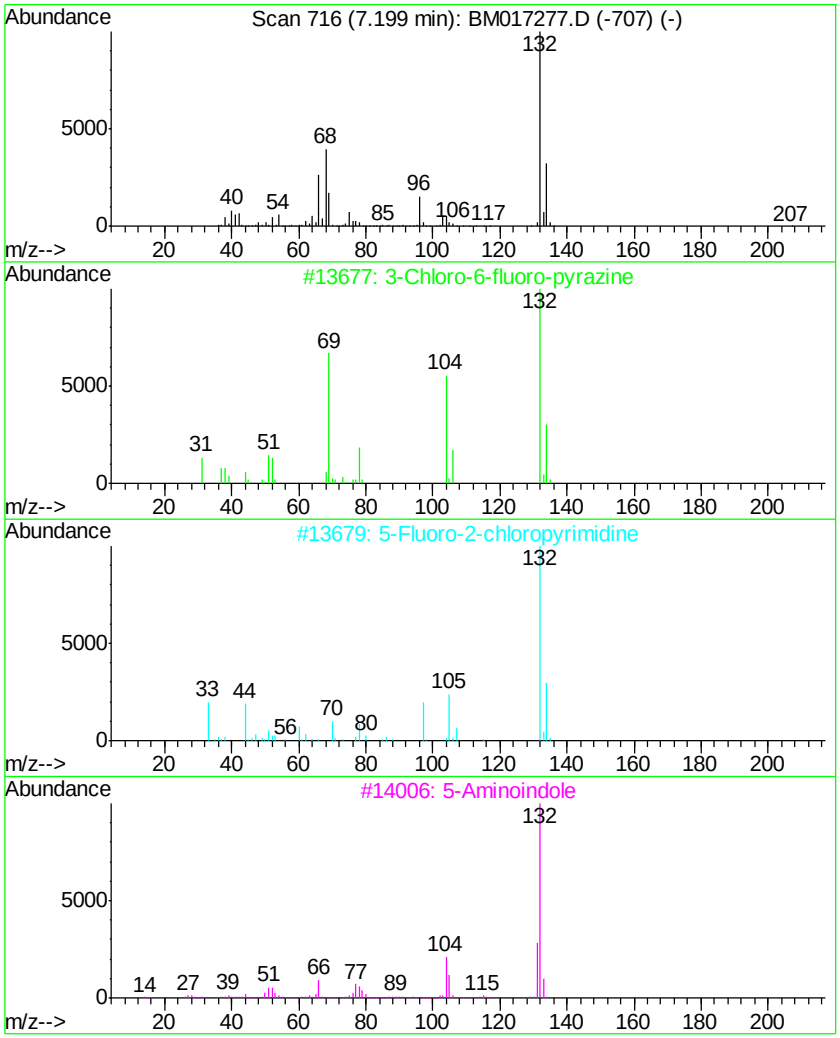
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

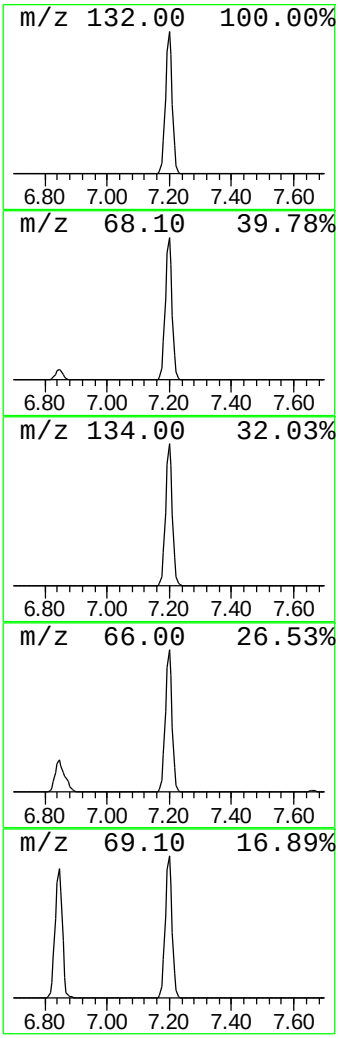
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	77.18 ng	7521740	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102218\
Data File : BM017277.D
Acq On : 22 Oct 2018 13:53
Operator : MJ/SJ
Sample : J5575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SSSI-1015-S-DH-24-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

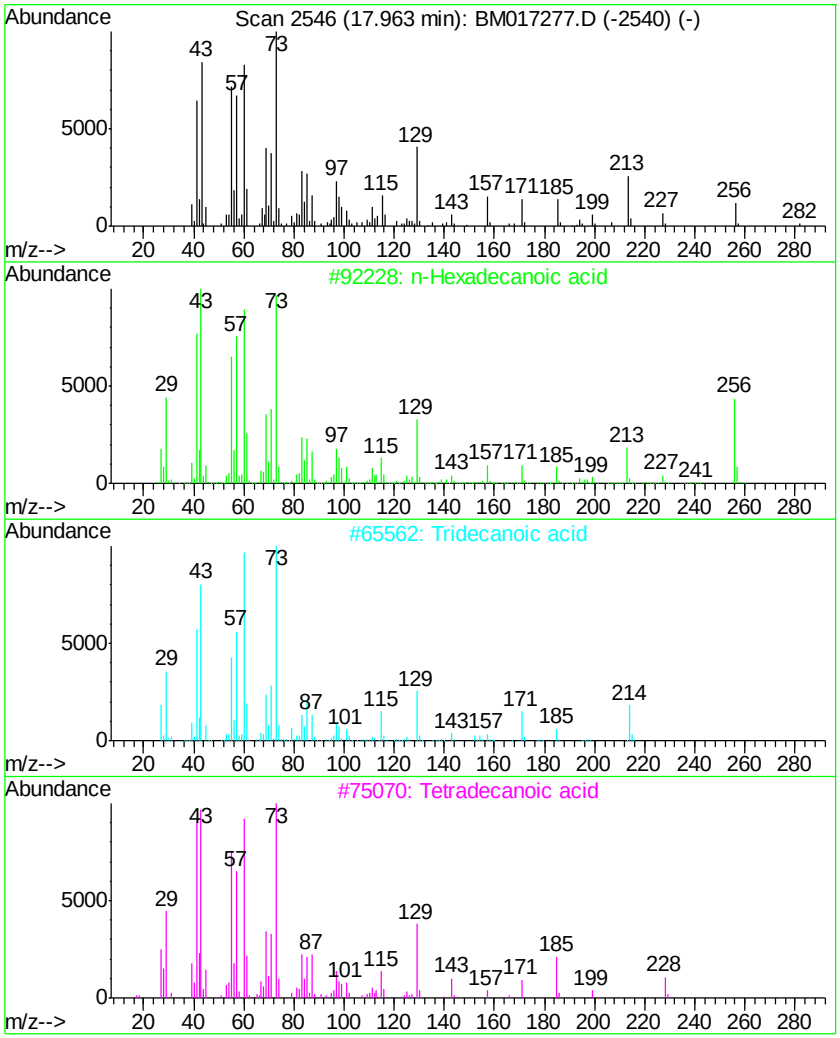
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

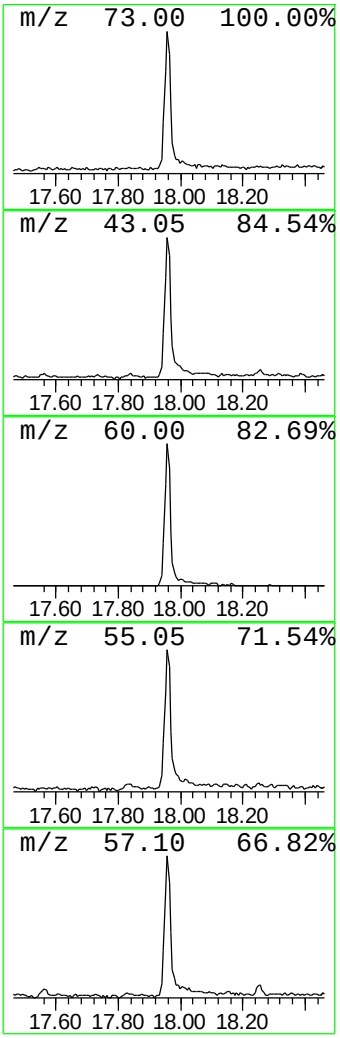
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	2.49 ng	535933	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102218\
Data File : BM017277.D
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Operator : MJ/SJ
Sample : J5575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SSSI-1015-S-DH-24-B

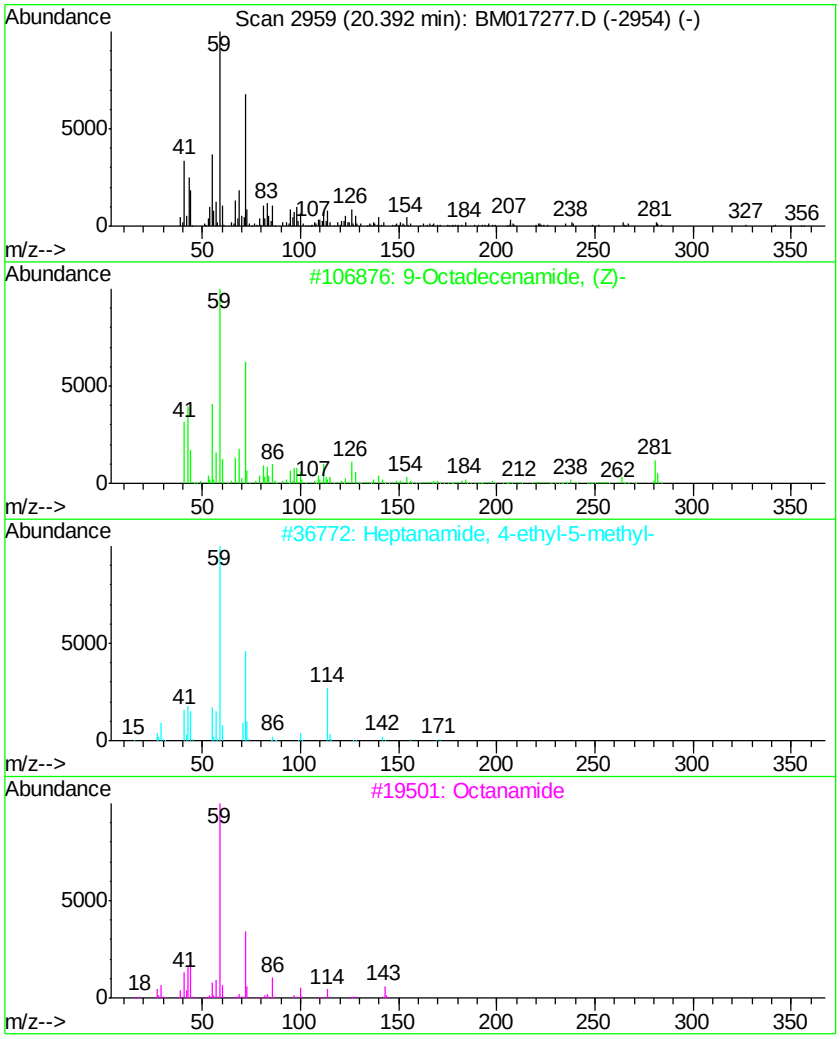
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

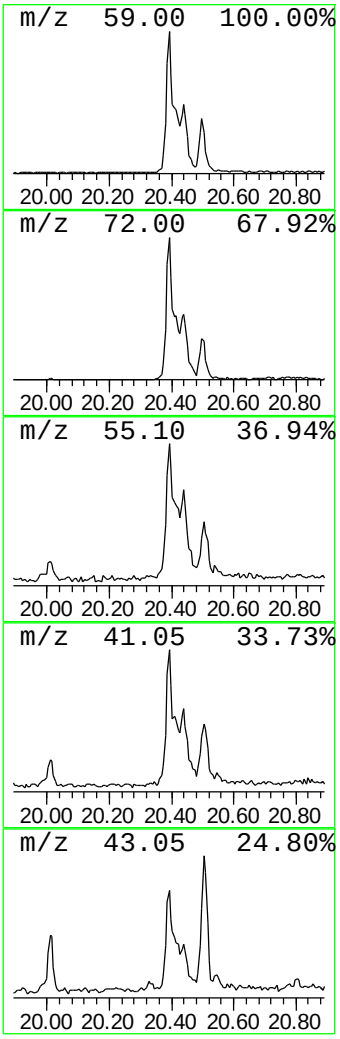
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.39	2.08 ng	491464	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
3	Octanamide	143	C8H17NO	000629-01-6	59
4	Decanamide-	171	C10H21NO	002319-29-1	59
5	Nonanamide	157	C9H19NO	001120-07-6	59





Library Search Compound Report

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ClientSampleId :
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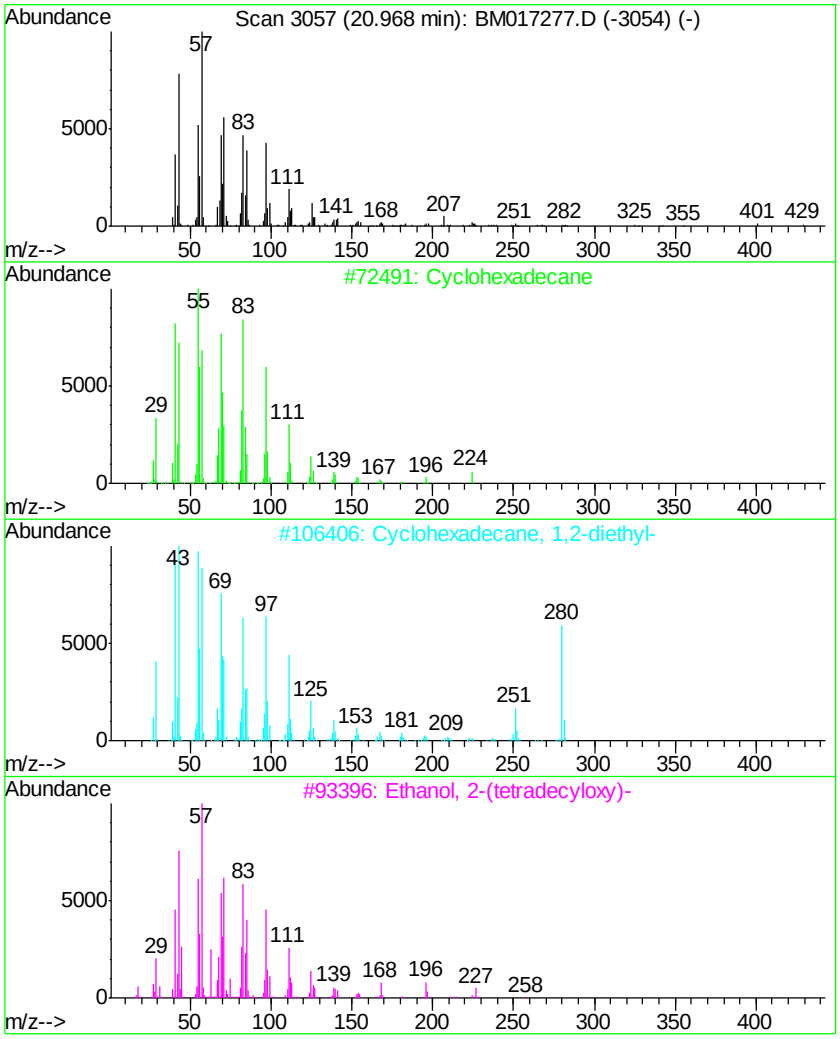
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

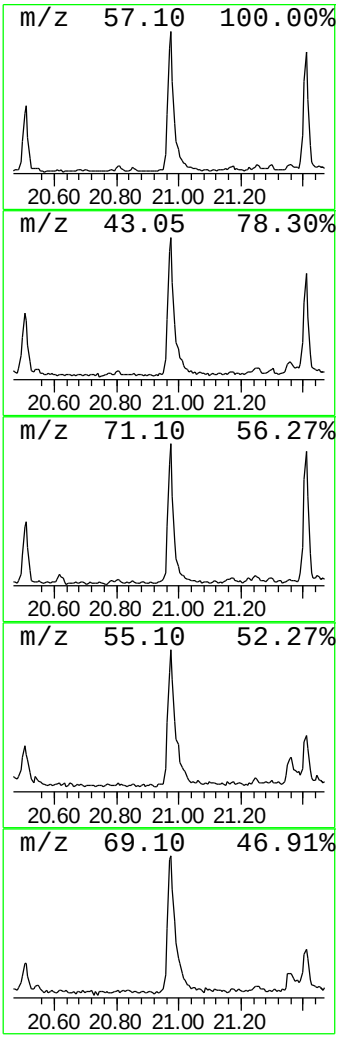
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	2.85 ng	672923	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	91
2	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	76
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	76





Library Search Compound Report

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BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

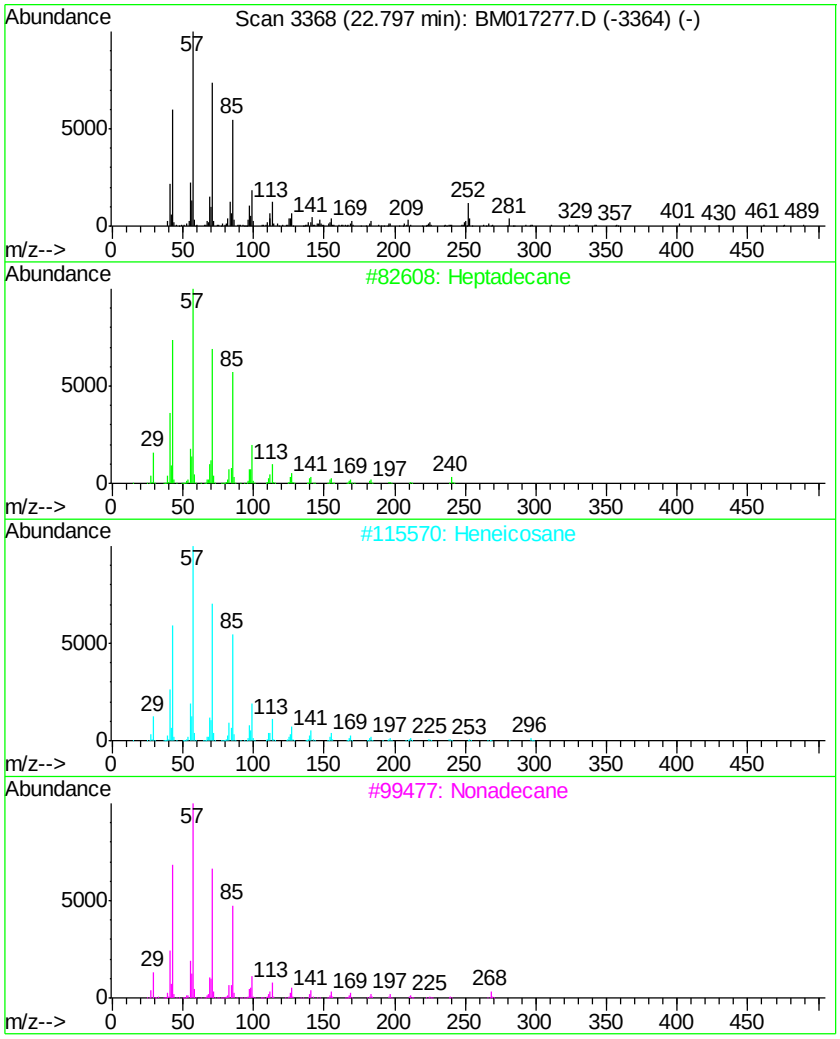
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

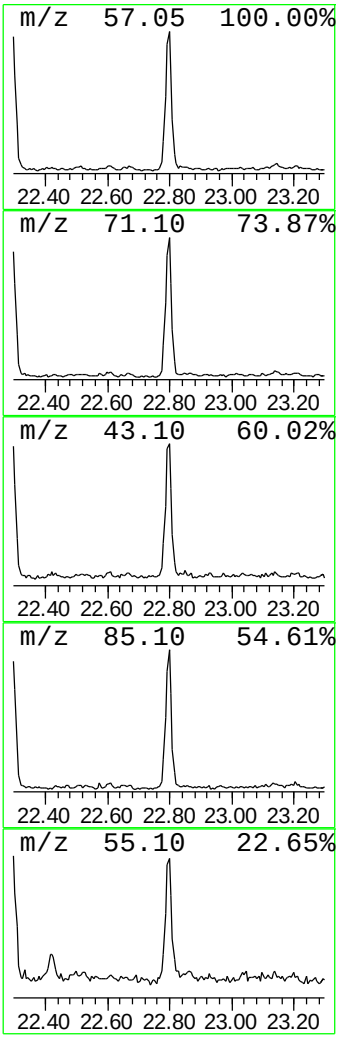
****

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.80	2.12 ng	422627	Perylene-d12	23.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	96
2	Heneicosane	296	C21H44	000629-94-7	96
3	Nonadecane	268	C19H40	000629-92-5	94
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	2.8	ng	277023	1	7.66	1949050	20.0
unknown7.20	7.20	77.2	ng	7521740	1	7.66	1949050	20.0
n-Hexadecanoic acid	17.96	2.5	ng	535933	4	17.05	4311160	20.0
9-Octadecenamide,...	20.39	2.1	ng	491464	5	21.24	4726270	20.0
Cyclohexadecane	20.97	2.9	ng	672923	5	21.24	4726270	20.0
Heptadecane	22.80	2.1	ng	422627	6	23.46	3980110	20.0