LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.034	492	501	510	rBV	117891	166368	5.02%	0.631%
2	5.428	562	568	571	rBV	2938853	3312094	100.00%	12.554%
3	5.751	620	623	629	rBV	52439	48238	1.46%	0.183%
4	6.028	668	670	673	rBV	44319	38721	1.17%	0.147%
5	6.063	673	676	689	rVB	119535	186591	5.63%	0.707%
6	6.445	734	741	743	rBV	2779605	3174949	95.86%	12.034%
7	6.581	759	764	767	rBV	3261594	3257427	98.35%	12.347%
8	6.810	799	803	806	rVB	870019	685440	20.70%	2.598%
9	6.969	825	830	833	rBV	2655126	2514510	75.92%	9.531%
10	7.375	893	899	902	rBV	2064389	1976625	59.68%	7.492%
11	8.092	1017	1021	1024	rBV	1023946	818975	24.73%	3.104%
12	9.169	1199	1204	1207	rBV	3203424	2808261	84.79%	10.644%
13	9.557	1267	1270	1273	rBV	265305	217682	6.57%	0.825%
14	9.774	1304	1307	1310	rVB	69995	48985	1.48%	0.186%
15	9.845	1315	1319	1323	rBV	849195	708484	21.39%	2.685%
16	10.274	1389	1392	1395	rVB	86414	64306	1.94%	0.244%
17	10.639	1449	1454	1457	rBV	1546217	1506342	45.48%	5.710%
18	10.751	1470	1473	1482	rBV	62458	68872	2.08%	0.261%
19	11.333	1568	1572	1575	rBV	786120	625776	18.89%	2.372%
20	11.857	1658	1661	1670	rBV2	116723	112918	3.41%	0.428%
21	12.545	1775	1778	1786	rBV	37653	37187	1.12%	0.141%
22	12.774	1813	1817	1822	rVB	36186	34614	1.05%	0.131%
23	12.927	1838	1843	1846	rBV	2404877	2307365	69.66%	8.746%
24	13.815	1991	1994	1998	rBV	114064	111535	3.37%	0.423%
25	13.980	2014	2022	2025	rBV	871003	870966	26.30%	3.301%
26	14.833	2164	2167	2172	rBV	54080	51428	1.55%	0.195%
27	15.445	2265	2271	2274	rBV	482394	627816	18.96%	2.380%

Sum of corrected areas: 26382475

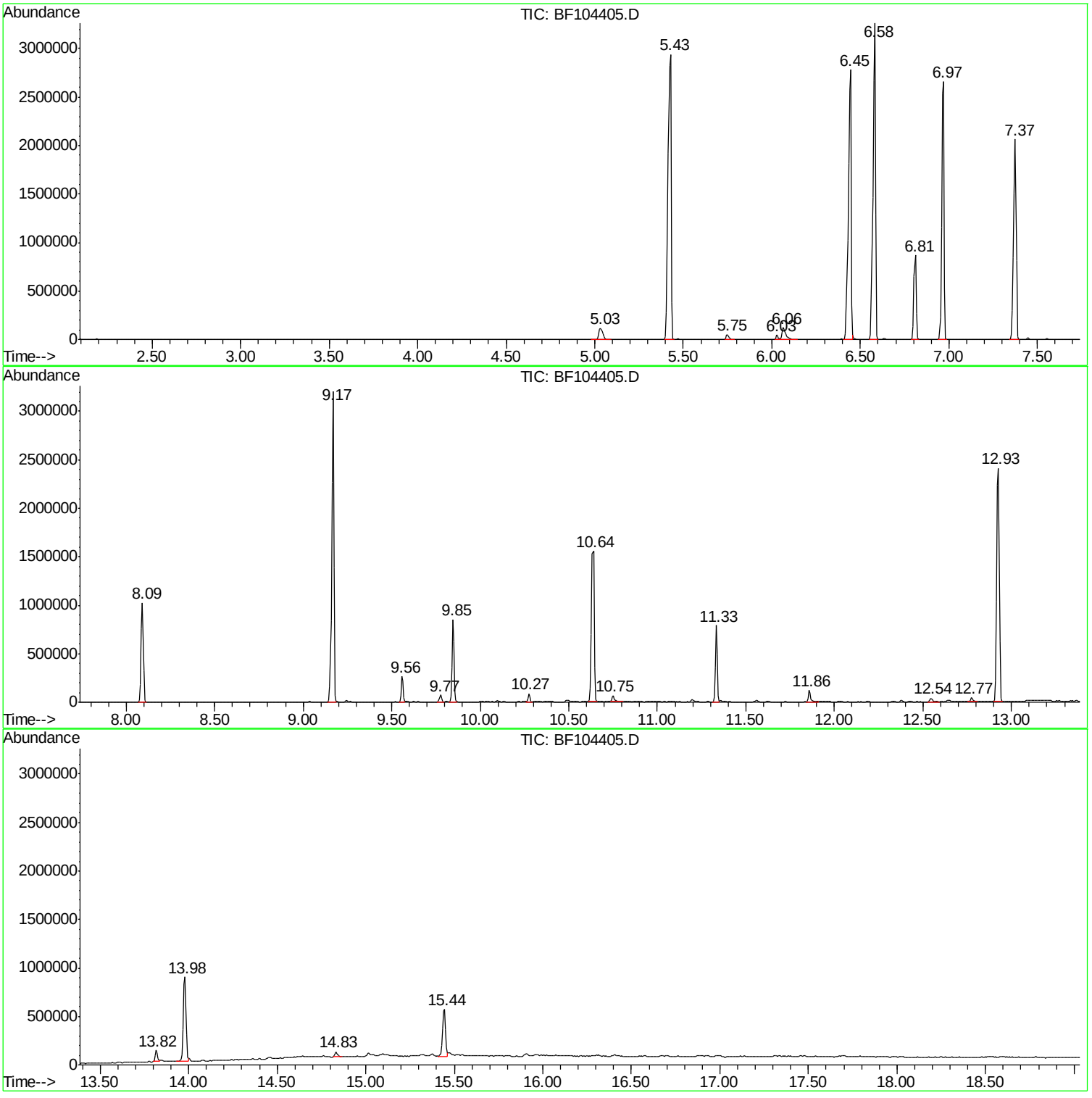
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

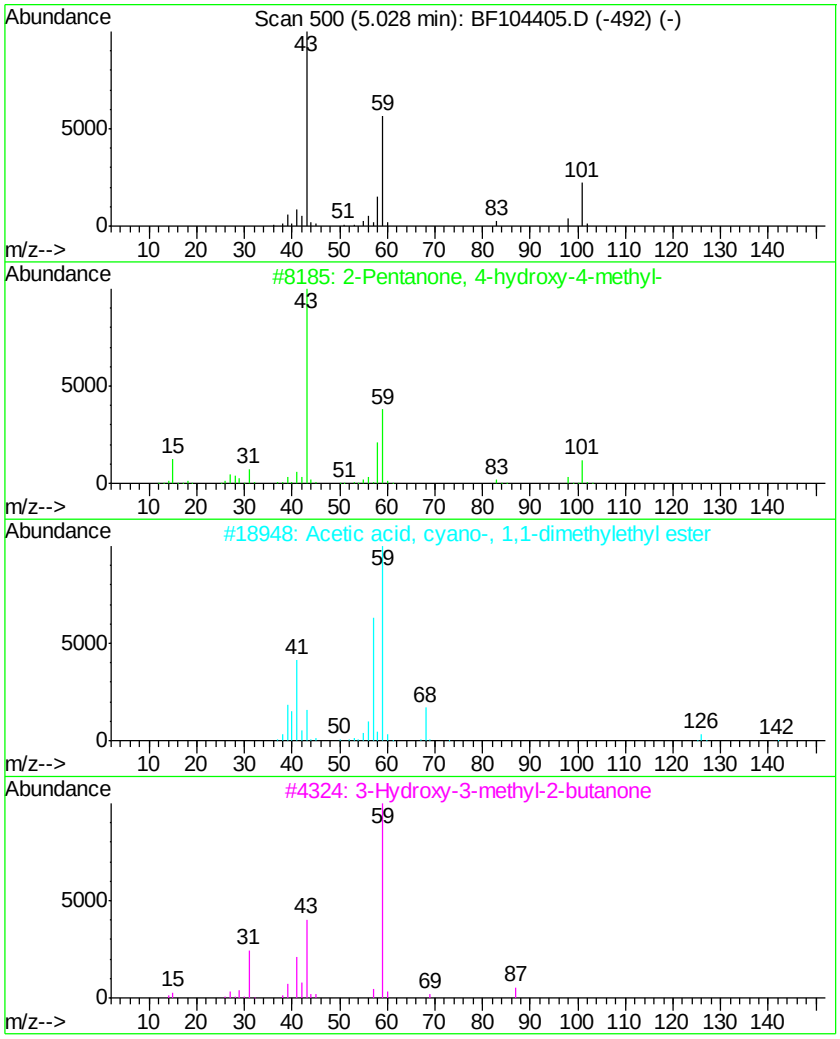
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

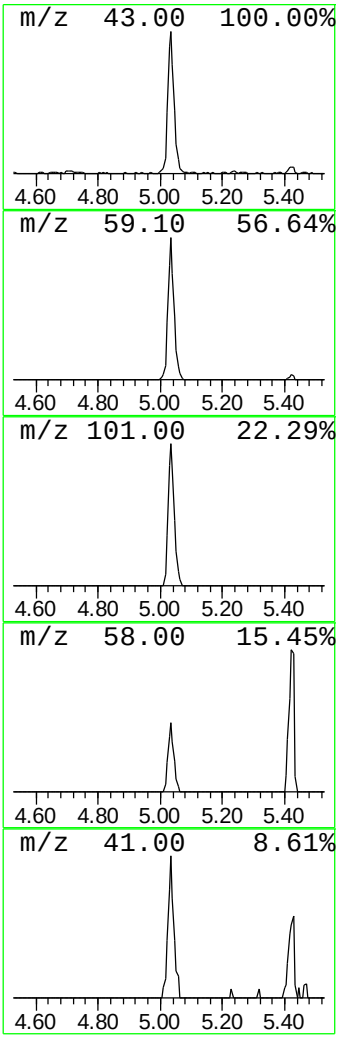
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	4.85 ng	166368	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

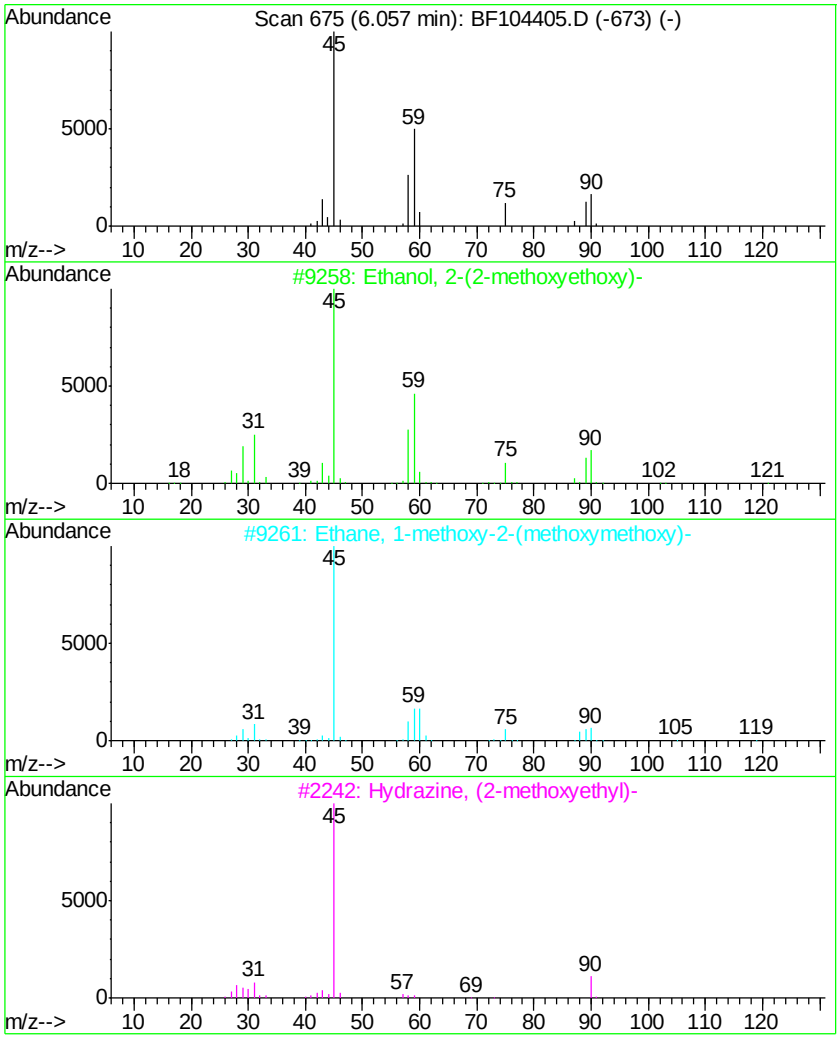
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

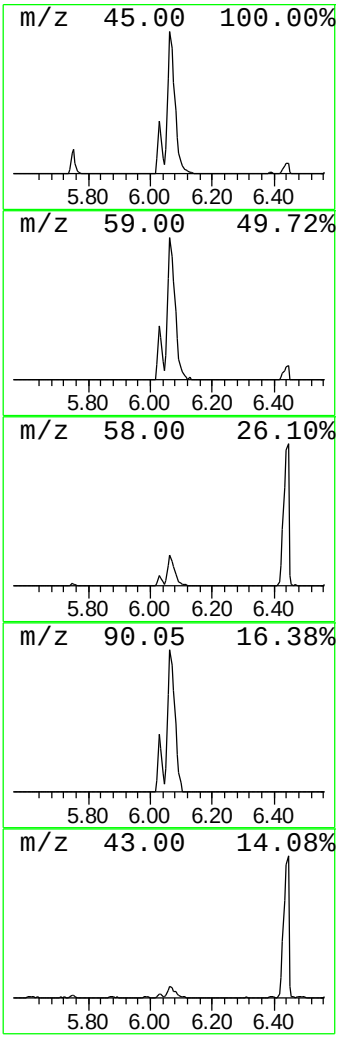
****

Peak Number 2 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.06	5.44 ng	186591	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	90
2	Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	38
3	Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	32
4	1,4-Dioxan-2-ol	104	C4H8O3	022347-47-3	28
5	Dimethyl-cyano-phosphine	87	C3H6NP	031641-57-3	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

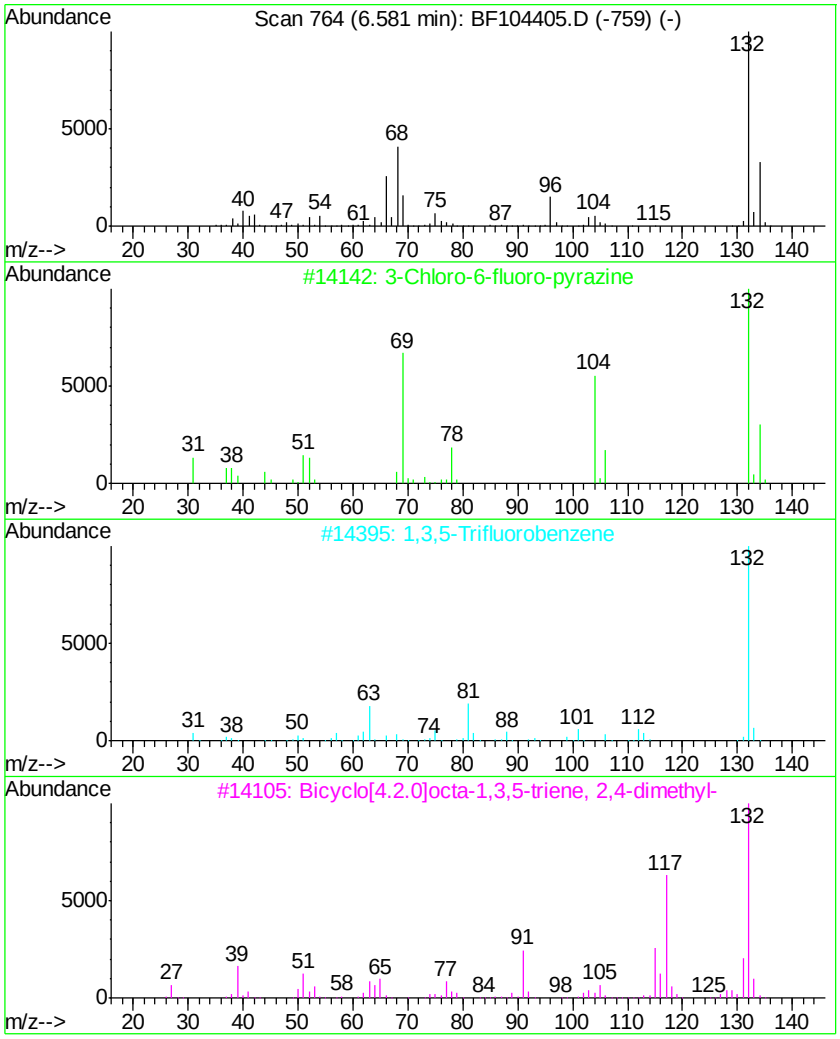
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

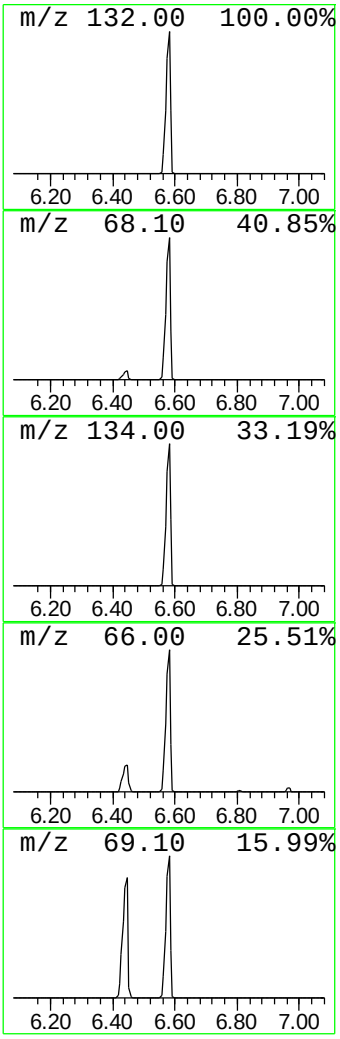
****

Peak Number 3 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	95.05 ng	3257430	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

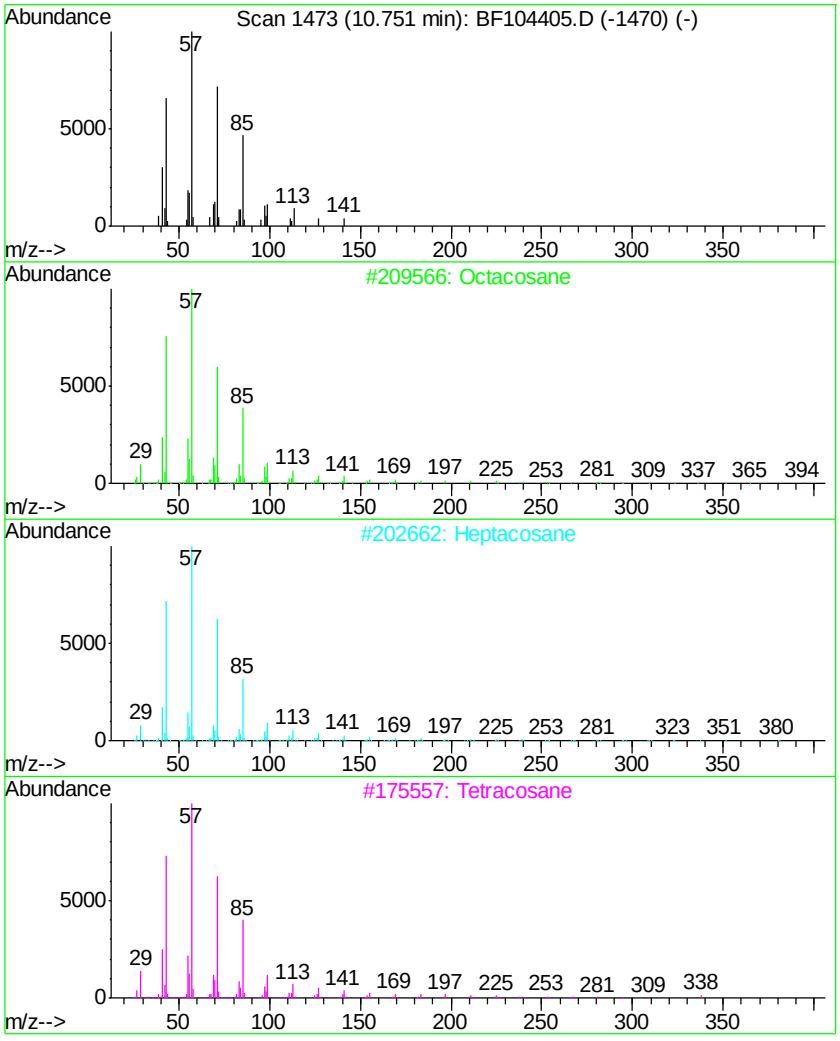
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

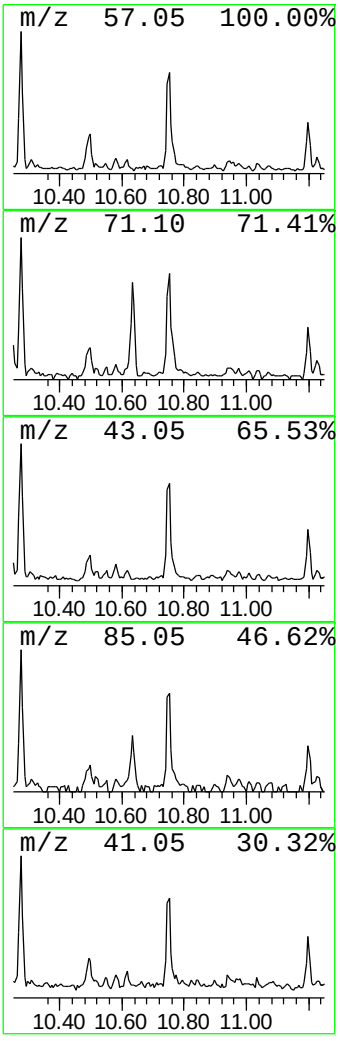
****

Peak Number 5 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.20 ng	68872	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	90
3	Tetracosane	338	C24H50	000646-31-1	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Hexadecane	226	C16H34	000544-76-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

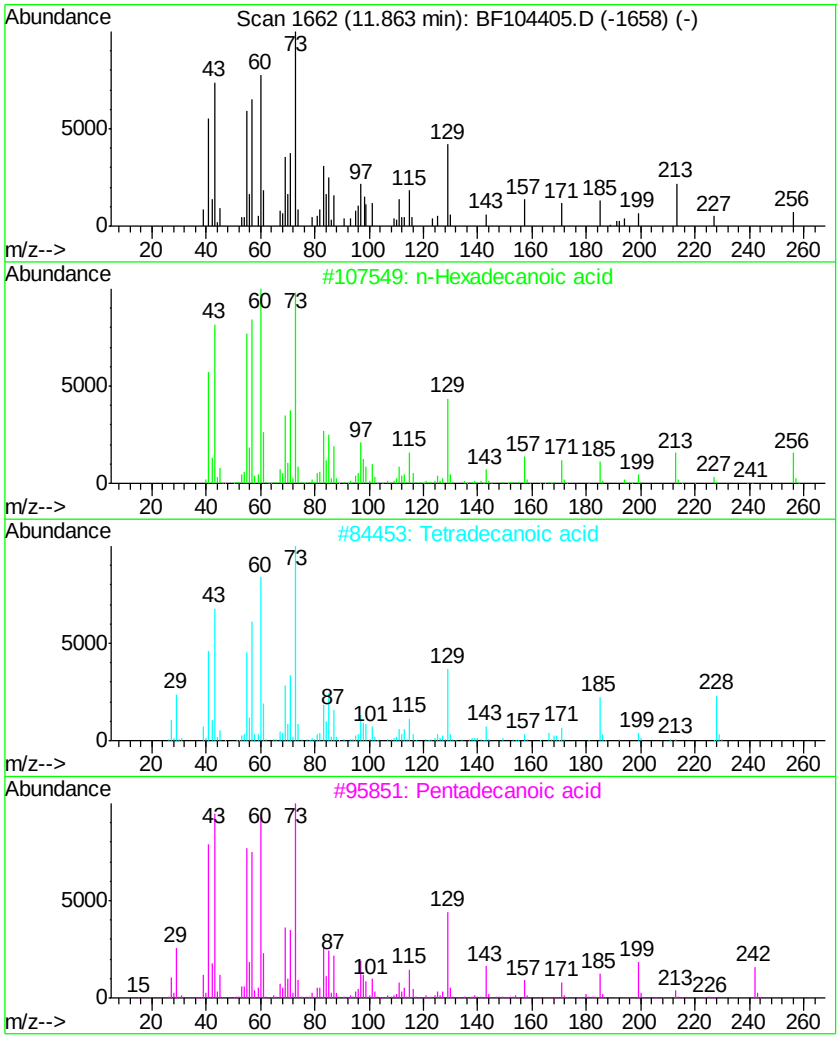
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

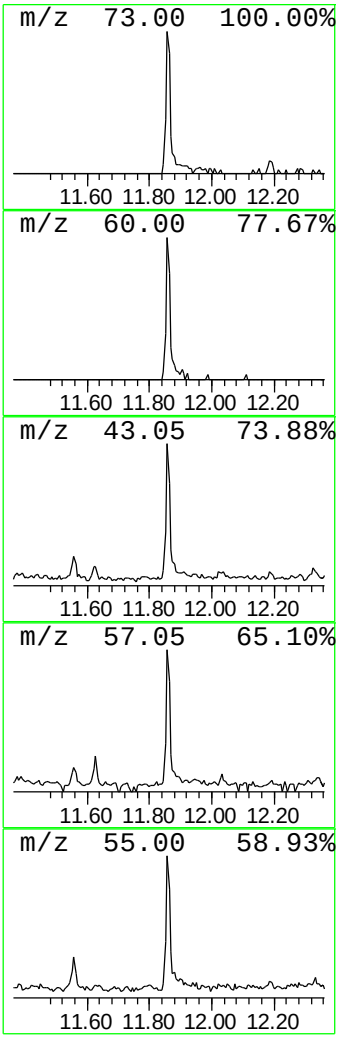
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	3.61 ng	112918	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

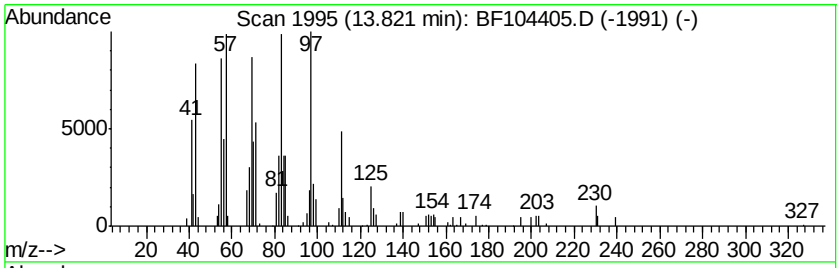
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

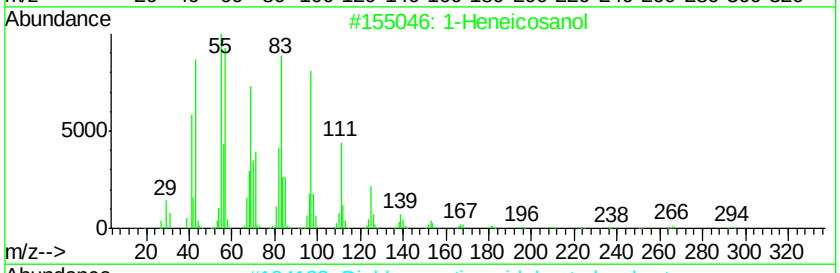
****

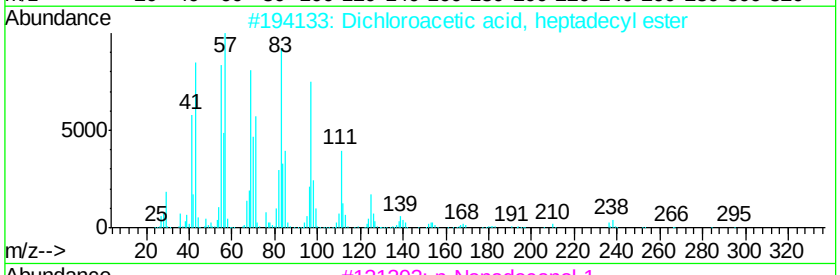
Peak Number 7 1-Heneicosanol Concentration Rank 6

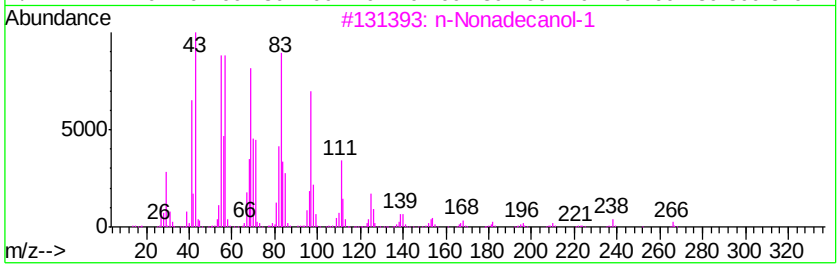
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.56 ng	111535	Chrysene-d12	13.98

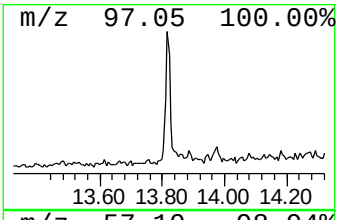
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94

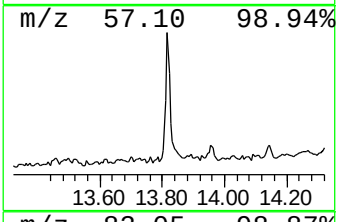


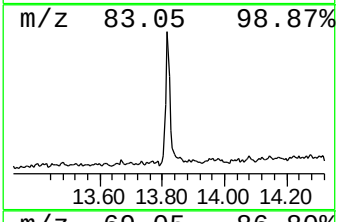


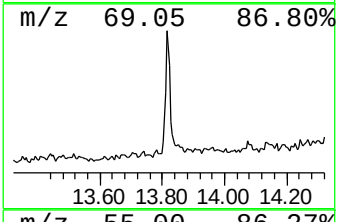


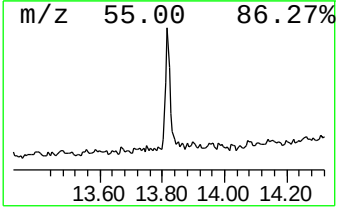












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041018\
Data File : BF104405.D
Acq On : 10 Apr 2018 13:42
Operator : JU/SJ
Sample : J2280-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	5.03	4.8	ng	166368	1	6.81	685440	20.0
Ethanol, 2-(2-met...	6.06	5.4	ng	186591	1	6.81	685440	20.0
unknown6.58	6.58	95.0	ng	3257430	1	6.81	685440	20.0
Octacosane	10.75	2.2	ng	68872	4	11.33	625776	20.0
n-Hexadecanoic acid	11.86	3.6	ng	112918	4	11.33	625776	20.0
1-Heneicosanol	13.82	2.6	ng	111535	5	13.98	870966	20.0