LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

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-BF050916.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	1.736	12	13	64	rVB	3227704	6711081	100.00%	18.182%
2	4.742	274	276	290	rBV	248249	422480	6.30%	1.145%
3	5.210	315	317	329	rBV	1343821	1919923	28.61%	5.202%
4	5.610	349	352	360	rVB	46888	79793	1.19%	0.216%
5	6.285	409	411	418	rBV	989948	1176581	17.53%	3.188%
6	6.387	418	420	425	rVB	3393053	3363983	50.13%	9.114%
7	6.605	437	439	445	rVB	693951	892884	13.30%	2.419%
8	6.765	451	453	456	rBV	3204132	2854255	42.53%	7.733%
9	7.153	482	487	488	rBV3	37147	72975	1.09%	0.198%
10	7.187	488	490	492	rBV	2813533	2734495	40.75%	7.408%
11	7.896	550	552	560	rVV	1213803	1200432	17.89%	3.252%
12	8.353	588	592	593	rBV3	29517	67981	1.01%	0.184%
13	8.925	641	642	644	rVB2	62794	69595	1.04%	0.189%
14	8.982	644	647	649	rBV	4044915	4471461	66.63%	12.114%
15	9.325	674	677	678	rBV3	42095	86603	1.29%	0.235%
16	9.382	680	682	683	rBV	91760	81836	1.22%	0.222%
17	9.645	702	705	707	rBV	1324103	1269258	18.91%	3.439%
18	10.011	735	737	740	rVV2	89891	113207	1.69%	0.307%
19	10.091	742	744	745	rVB2	78750	88824	1.32%	0.241%
20	10.434	772	774	777	rBV2	2178669	2586797	38.55%	7.008%
21	10.491	777	779	783	rVV2	56527	120810	1.80%	0.327%
22	10.559	783	785	789	rVB	68555	112233	1.67%	0.304%
23	11.119	832	834	837	rBV	1032598	1062970	15.84%	2.880%
24	11.679	881	883	888	rVB4	127572	205666	3.06%	0.557%
25	12.457	949	951	953	rBV	66301	76866	1.15%	0.208%
26	12.491	953	954	957	rVB	75469	87251	1.30%	0.236%
27	12.537	957	958	961	rBV	55785	79184	1.18%	0.215%
28	12.708	970	973	976	rBV	3306937	3163549	47.14%	8.571%
29	13.611	1050	1052	1057	rBV	80639	137367	2.05%	0.372%
30	13.748	1062	1064	1067	rBV	821816	816670	12.17%	2.213%
31	15.108	1181	1183	1189	rBV	656463	783536	11.68%	2.123%

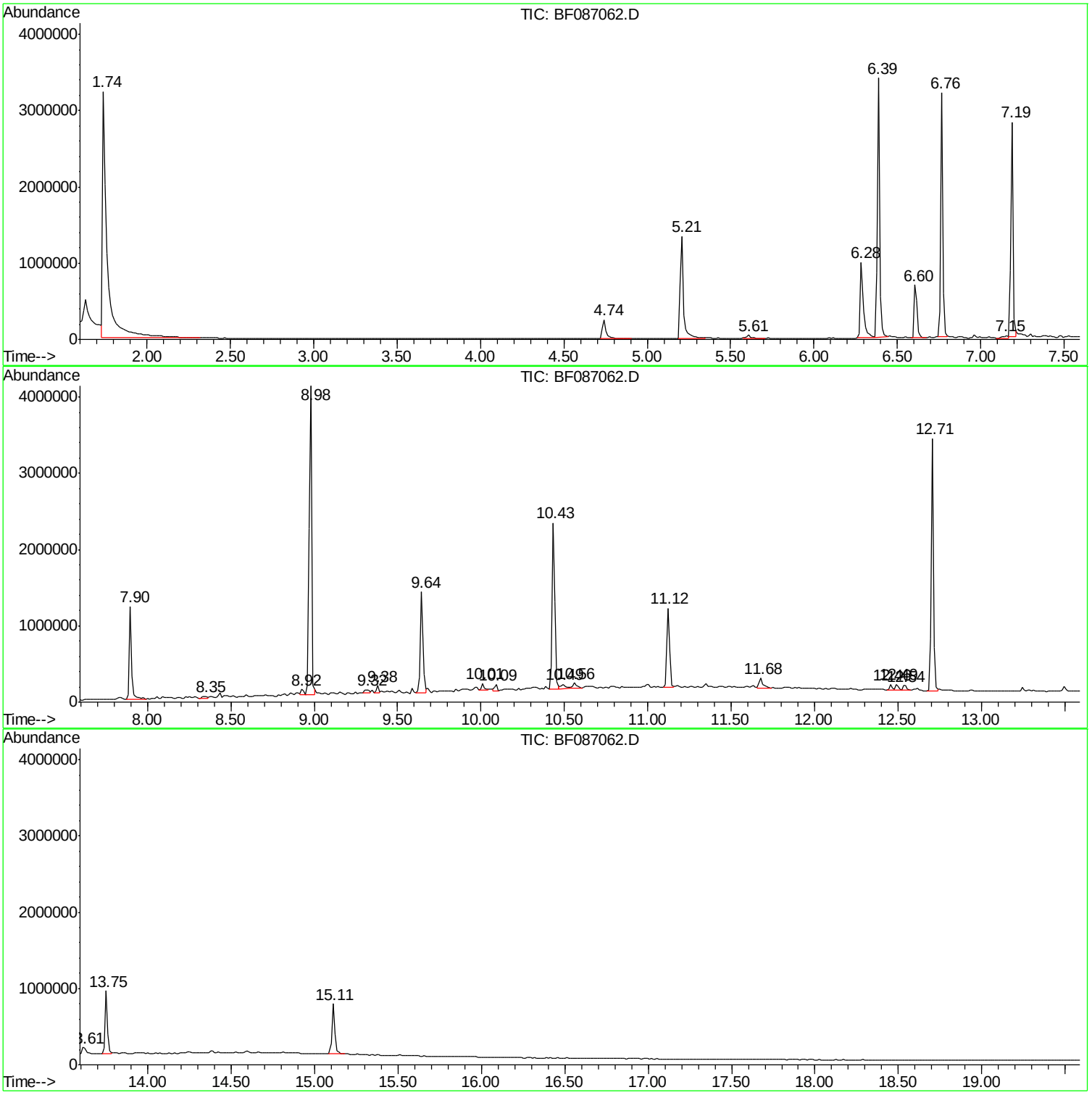
Sum of corrected areas: 36910546

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

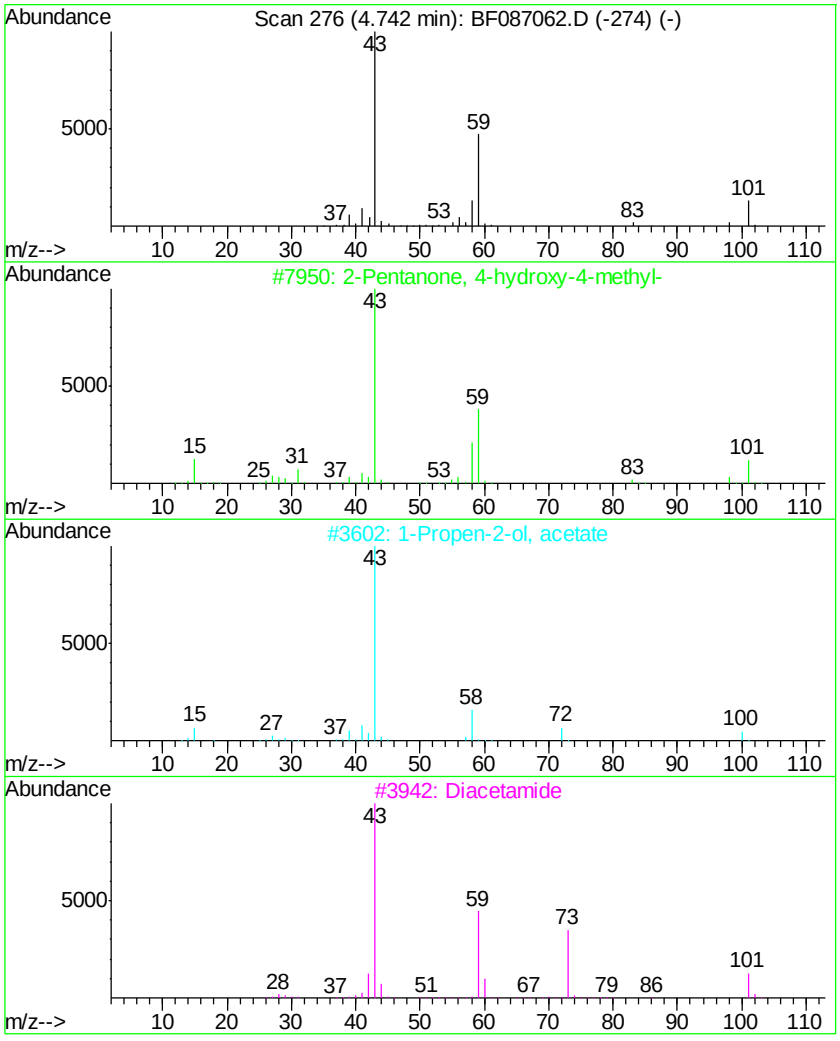
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

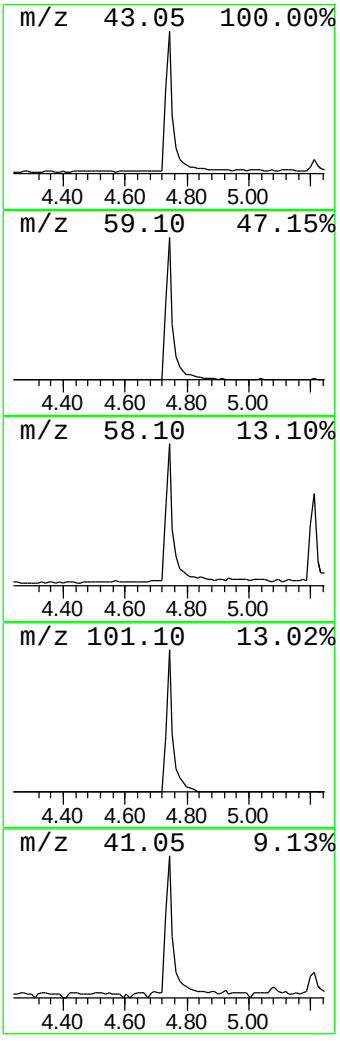
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	9.46 ng	422480	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	Butane	58	C4H10	000106-97-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

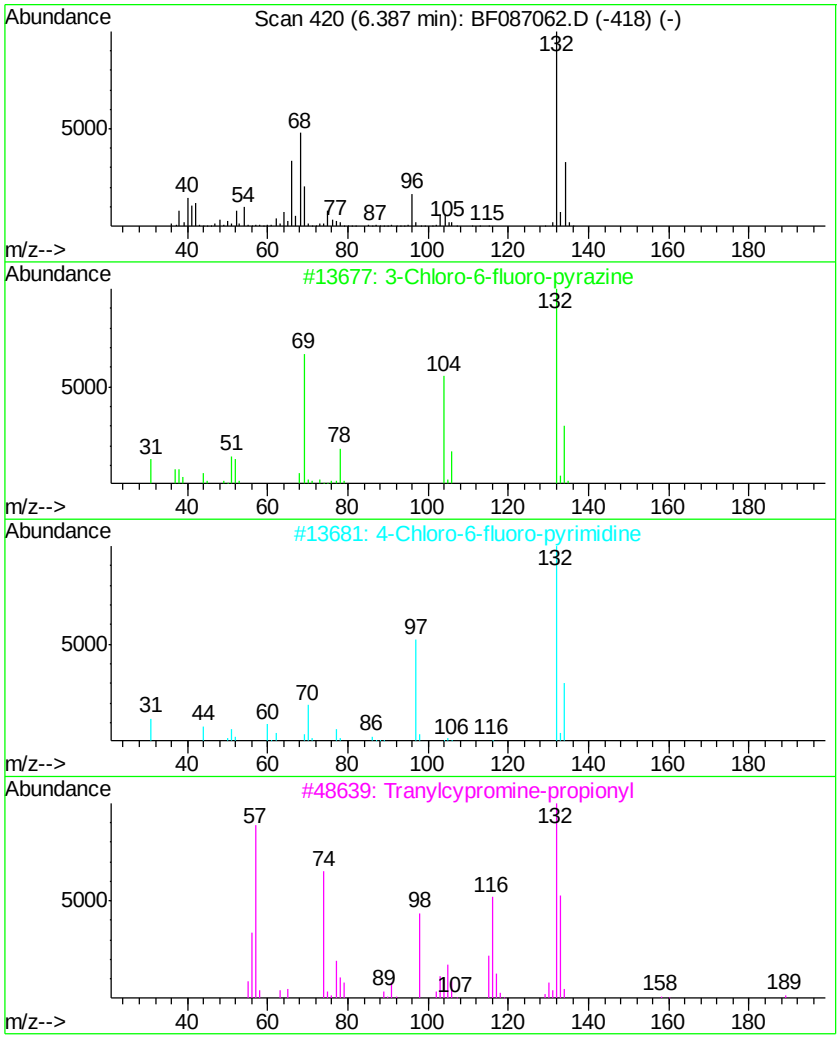
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

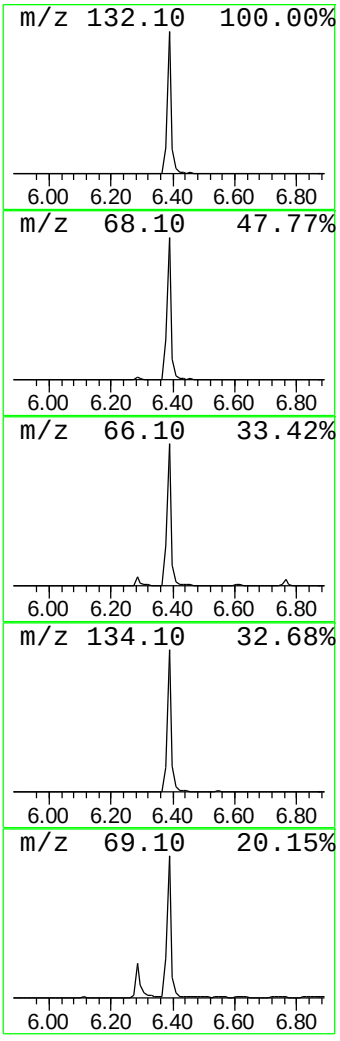
****

Peak Number 3 unknown6.39 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	75.35 ng	3363980	1,4-Dichlorobenzene-d4	6.60

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

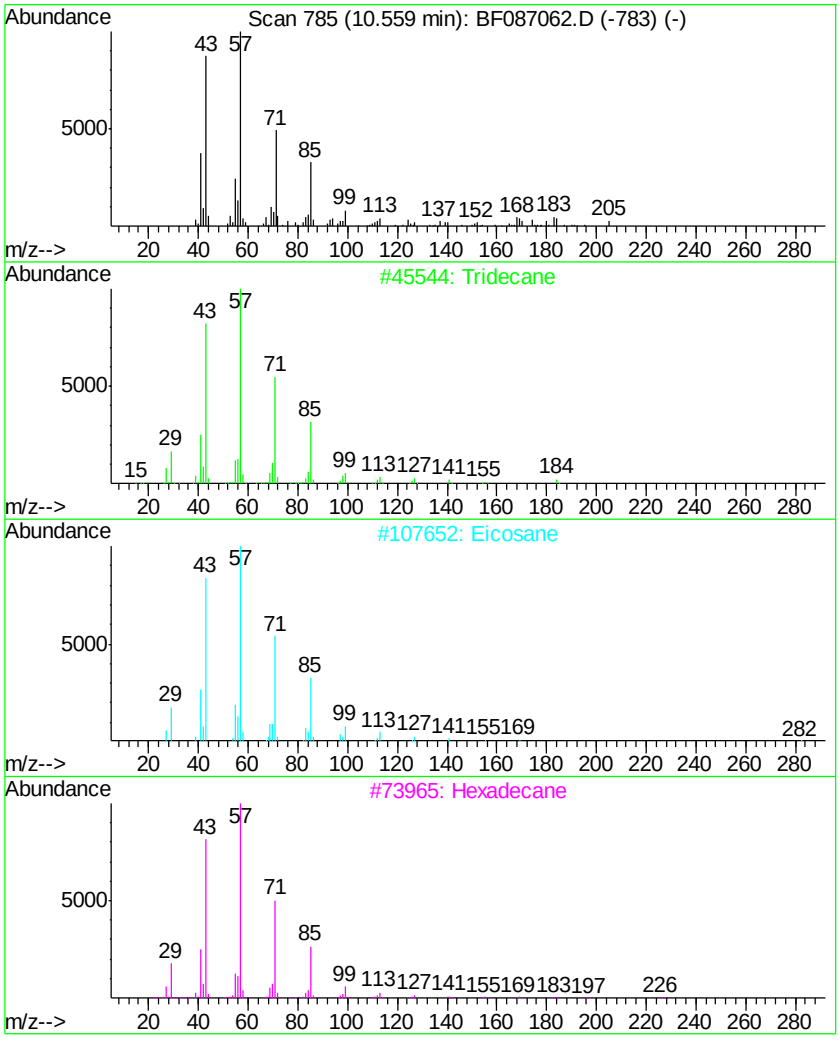
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

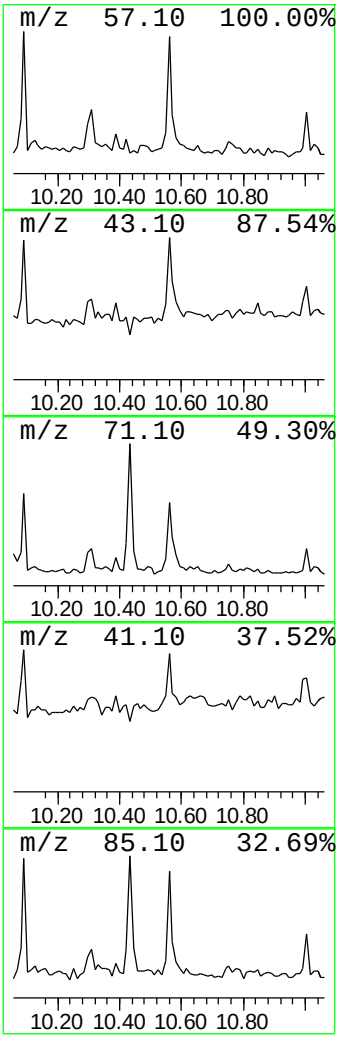
****

Peak Number 5 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.11 ng	112233	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	83
2	Eicosane	282	C20H42	000112-95-8	74
3	Hexadecane	226	C16H34	000544-76-3	74
4	Dodecane	170	C12H26	000112-40-3	74
5	5-Ethyldecane	170	C12H26	017302-36-2	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

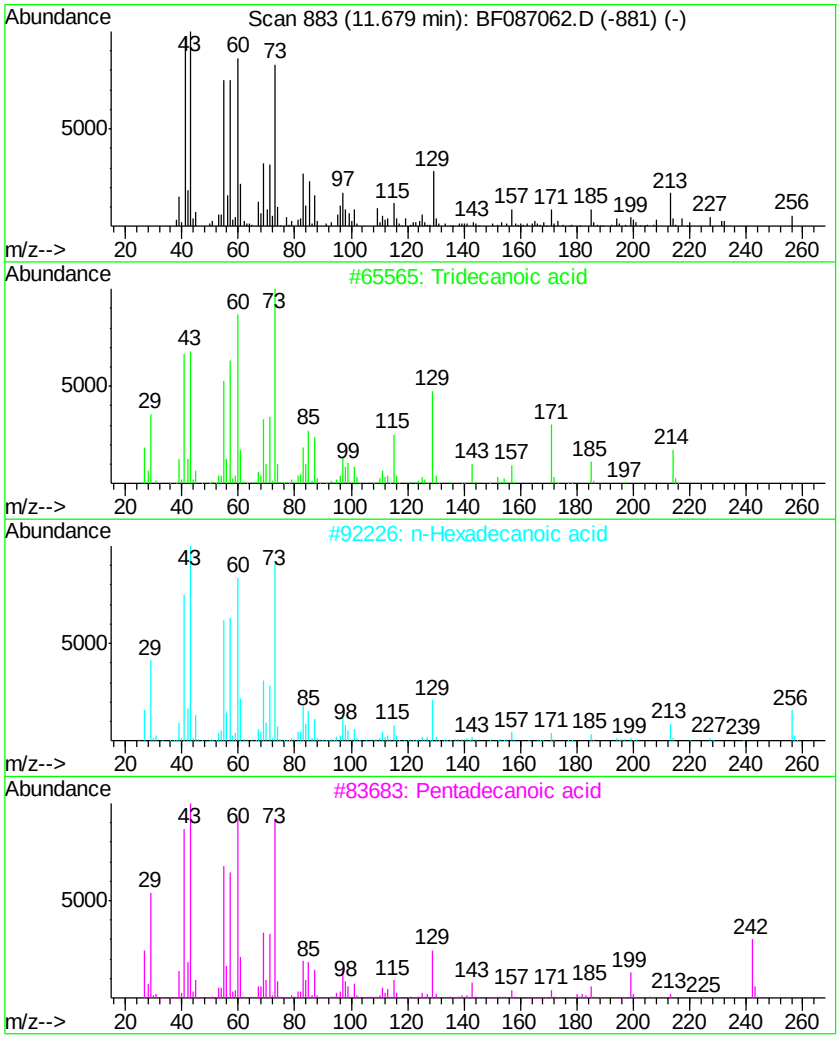
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

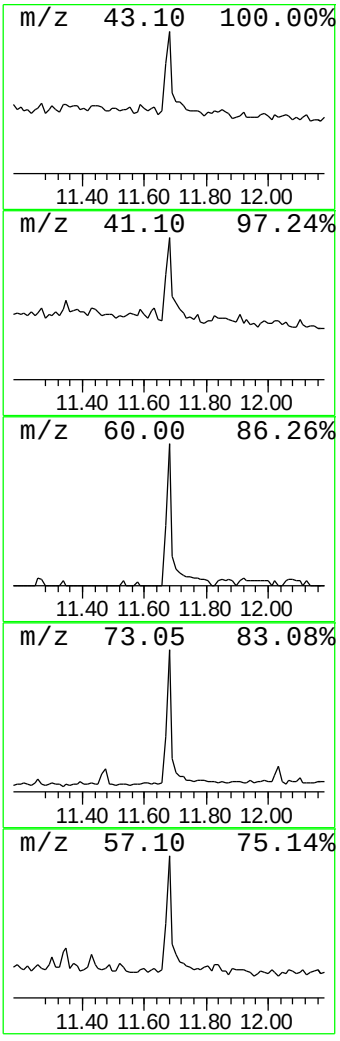
****

Peak Number 6 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	3.87 ng	205666	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

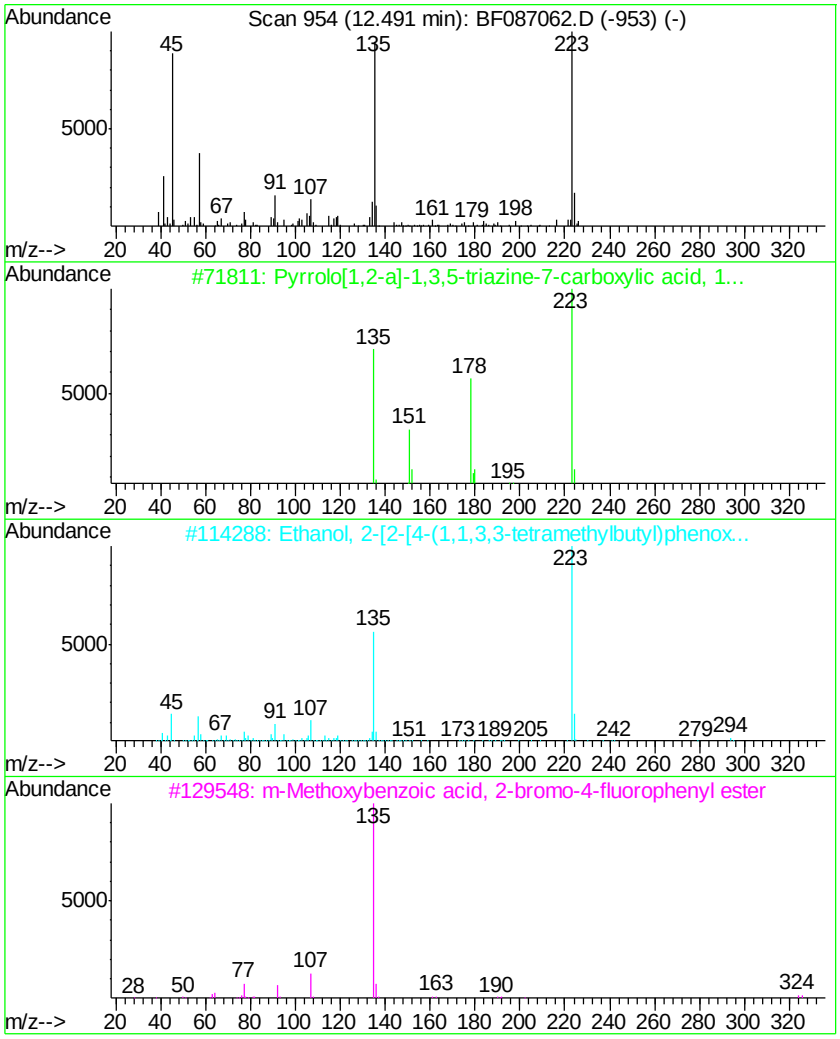
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

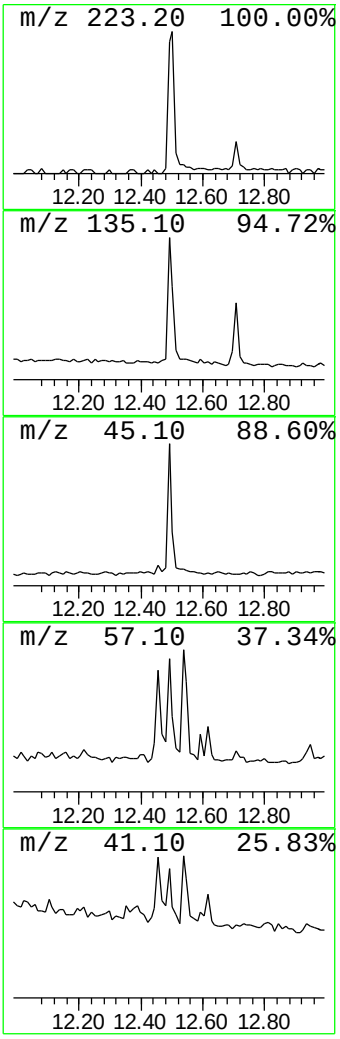
****

Peak Number 7 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	2.14 ng	87251	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	83
2	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	35
3	m-Methoxybenzoic acid, 2-bromo-4...	324	C14H10BrFO3	1000292-63-0	35
4	2-Propanone, 1-(2,5-dimethoxy-4-...	223	C12H17NO3	043021-99-4	25
5	4-Methoxybenzenamide, N-(4-ethox...	298	C17H18N2O3	303083-85-4	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

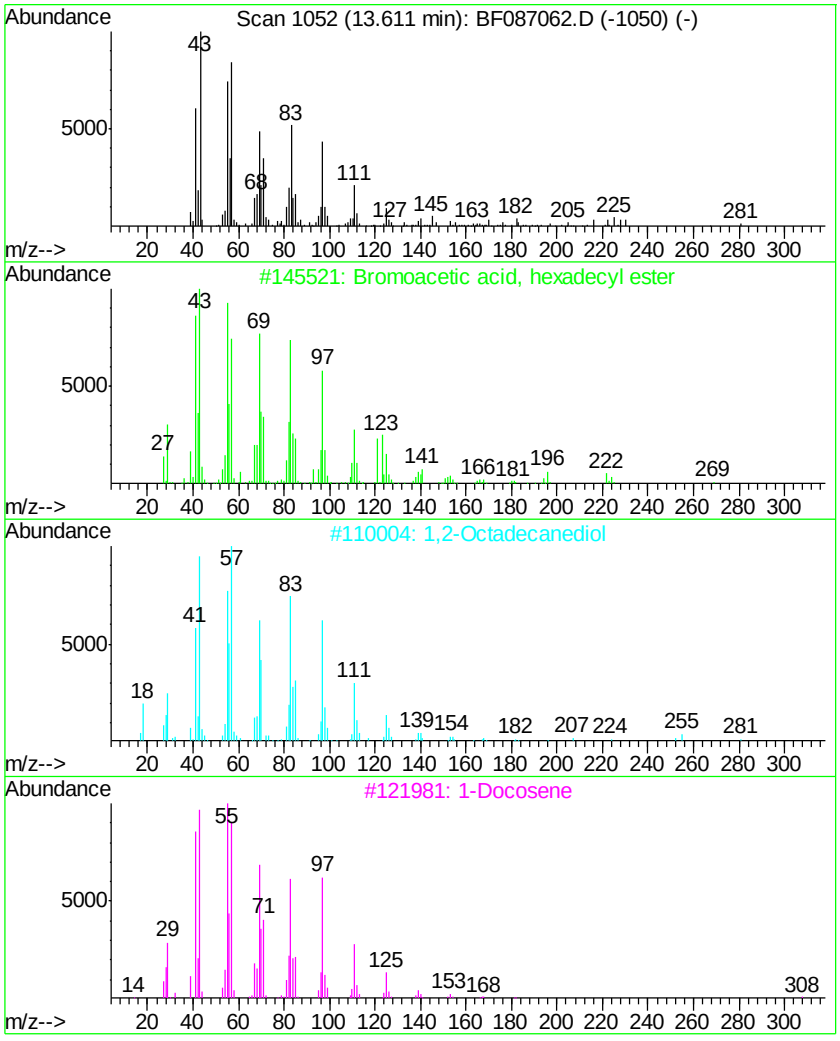
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

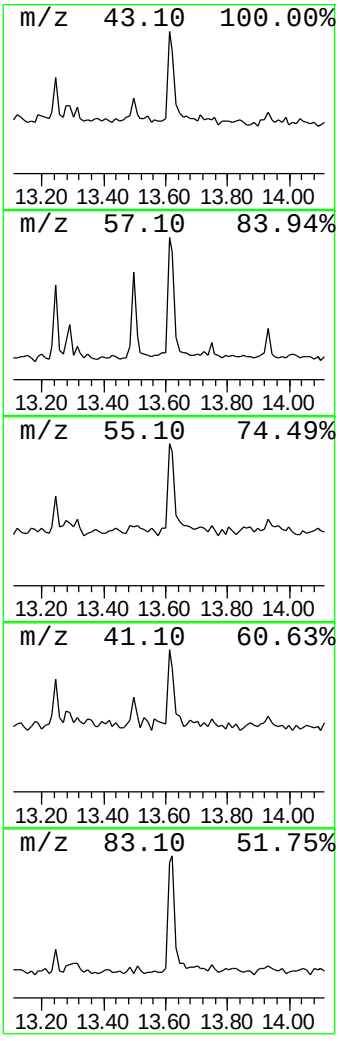
****

Peak Number 8 Bromoacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	3.36 ng	137367	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
2	1,2-Octadecanediol	286	C18H38O2	020294-76-2	87
3	1-Docosene	308	C22H44	001599-67-3	87
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087062.D
Acq On : 15 May 2016 11:36
Operator : UM/SJ
Sample : H3052-13
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.74	9.5	ng	422480	1	6.60	892884	20.0
unknown6.39	6.39	75.3	ng	3363980	1	6.60	892884	20.0
Tridecane	10.56	2.1	ng	112233	4	11.12	1062970	20.0
Tridecanoic acid	11.68	3.9	ng	205666	4	11.12	1062970	20.0
Pyrrolo[1,2-a]-1,...	12.49	2.1	ng	87251	5	13.75	816670	20.0
Bromoacetic acid,...	13.61	3.4	ng	137367	5	13.75	816670	20.0