LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF087800.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.667	4	7	10	rVB	3525435	4834062	100.00%	16.167%
2	1.758	14	15	25	rVV	271221	460956	9.54%	1.542%
3	1.896	25	27	41	rVB	1496796	2472562	51.15%	8.269%
4	2.067	41	42	59	rVB3	61212	197248	4.08%	0.660%
5	5.016	297	300	304	rBV	120445	169412	3.50%	0.567%
6	5.439	334	337	339	rBV	1129084	1610060	33.31%	5.385%
7	6.467	424	427	430	rBV	1528074	1491321	30.85%	4.987%
8	6.605	436	439	441	rBV	1834008	1663000	34.40%	5.562%
9	6.833	457	459	462	rBV	460928	541990	11.21%	1.813%
10	6.993	471	473	476	rVB	1534313	1294588	26.78%	4.330%
11	7.405	506	509	511	rVB	1060702	1158759	23.97%	3.875%
12	8.125	569	572	574	rBV	945651	834230	17.26%	2.790%
13	9.199	663	666	668	rBV	2312927	1996541	41.30%	6.677%
14	9.291	671	674	676	rVB2	43210	62849	1.30%	0.210%
15	9.588	698	700	703	rBV	203121	210589	4.36%	0.704%
16	9.736	711	713	718	rVB	161594	142426	2.95%	0.476%
17	9.873	722	725	727	rBV	1065140	909128	18.81%	3.040%
18	10.662	791	794	796	rBV	1027703	1237045	25.59%	4.137%
19	10.776	803	804	808	rBV	38476	68463	1.42%	0.229%
20	11.222	839	843	849	rVB3	33913	77789	1.61%	0.260%
21	11.348	852	854	859	rBV2	814266	1149398	23.78%	3.844%
22	11.428	859	861	862	rVB	67640	71787	1.49%	0.240%
23	11.874	899	900	902	rVV	52516	56818	1.18%	0.190%
24	11.965	906	908	912	rVB	63180	103518	2.14%	0.346%
25	12.148	921	924	928	rBV2	30846	53296	1.10%	0.178%
26	12.445	947	950	951	rBV2	47043	64601	1.34%	0.216%
27	12.479	951	953	956	rVB	91274	113144	2.34%	0.378%
28	12.559	957	960	962	rVB	473658	458764	9.49%	1.534%
29	12.651	967	968	970	rBV2	150240	120173	2.49%	0.402%
30	12.685	970	971	975	rVB2	151082	149751	3.10%	0.501%
31	12.788	975	980	981	rBV	349226	510387	10.56%	1.707%
32	12.937	991	993	995	rVB	1939296	1868640	38.66%	6.249%
33	13.108	1003	1008	1010	rVB2	57639	106478	2.20%	0.356%
34	13.177	1010	1014	1015	rBV	57529	65661	1.36%	0.220%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SS-1

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.611	1049	1052	1055	rBV2	29728	50355	1.04%	0.168%
36	13.862	1071	1074	1080	rVB3	49116	101368	2.10%	0.339%
37	13.977	1081	1084	1089	rVB2	818283	1113982	23.04%	3.726%
38	14.503	1127	1130	1132	rVB3	30430	56114	1.16%	0.188%
39	14.983	1169	1172	1177	rBV	152028	321556	6.65%	1.075%
40	15.085	1178	1181	1183	rVV2	63052	102722	2.12%	0.344%
41	15.143	1183	1186	1192	rVV5	24970	90761	1.88%	0.304%
42	15.268	1195	1197	1200	rVV	99116	125762	2.60%	0.421%
43	15.325	1200	1202	1205	rVV	117092	171248	3.54%	0.573%
44	15.394	1205	1208	1214	rVB	501456	691538	14.31%	2.313%
45	15.851	1245	1248	1251	rBV	76750	137846	2.85%	0.461%
46	16.068	1265	1267	1274	rVB5	26533	62414	1.29%	0.209%
47	16.480	1300	1303	1308	rVB4	24887	61085	1.26%	0.204%
48	16.766	1324	1328	1333	rVB2	51561	107954	2.23%	0.361%
49	17.177	1360	1364	1372	rVB	47948	107539	2.22%	0.360%
50	17.394	1379	1383	1390	rVB4	28974	98298	2.03%	0.329%
51	18.297	1458	1462	1471	rVB6	16827	61859	1.28%	0.207%
52	19.280	1543	1548	1556	rVB5	30803	113447	2.35%	0.379%

Sum of corrected areas: 29901282

LSC Report - Integrated Chromatogram

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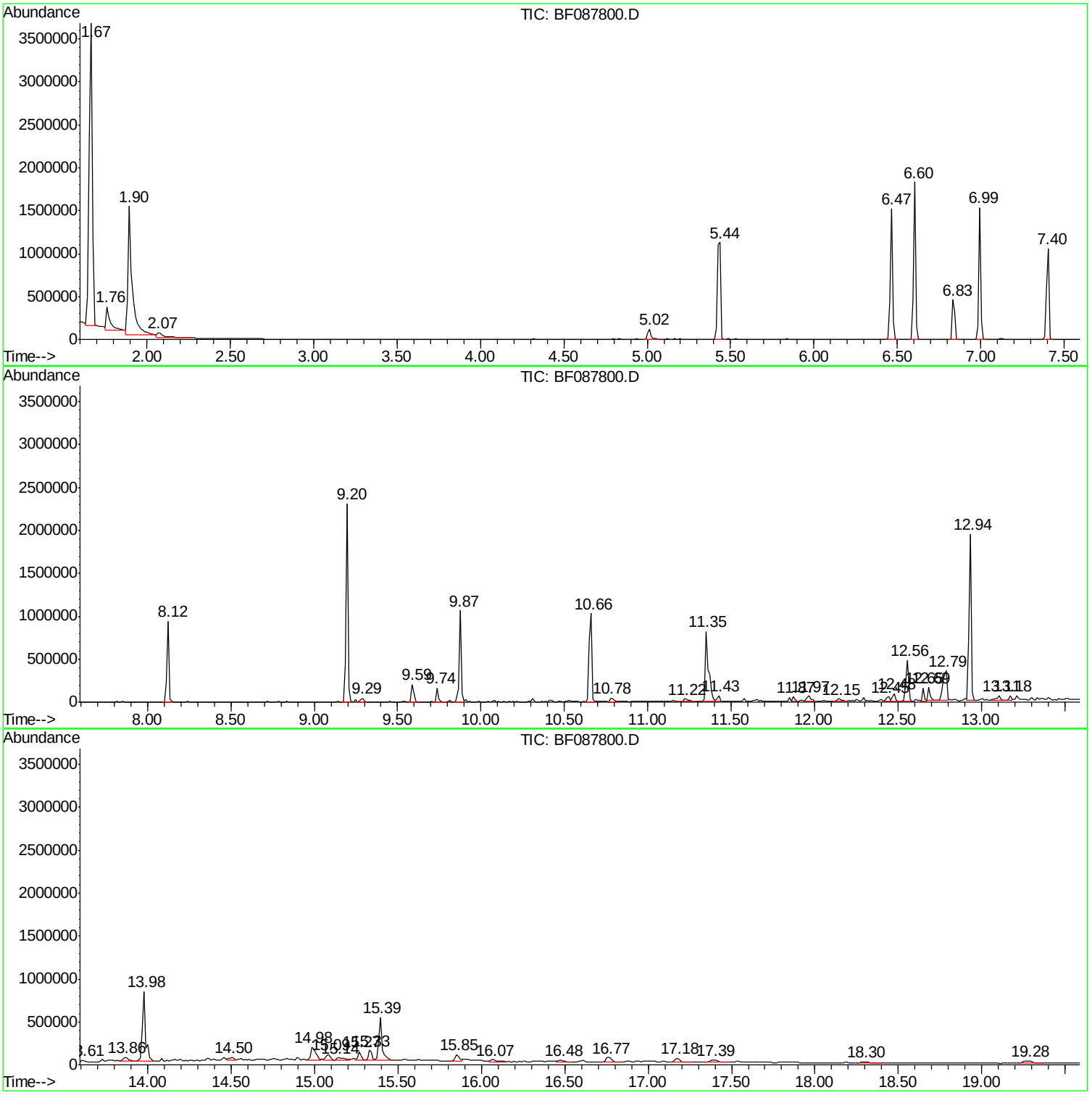
Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

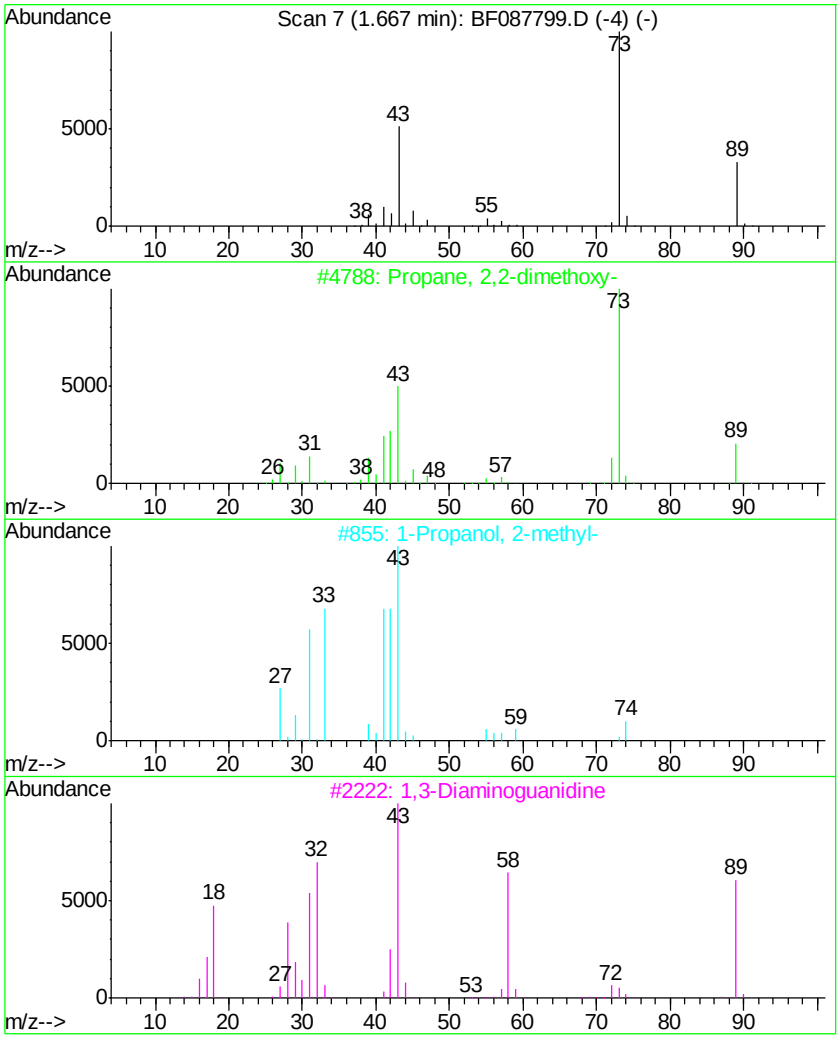
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

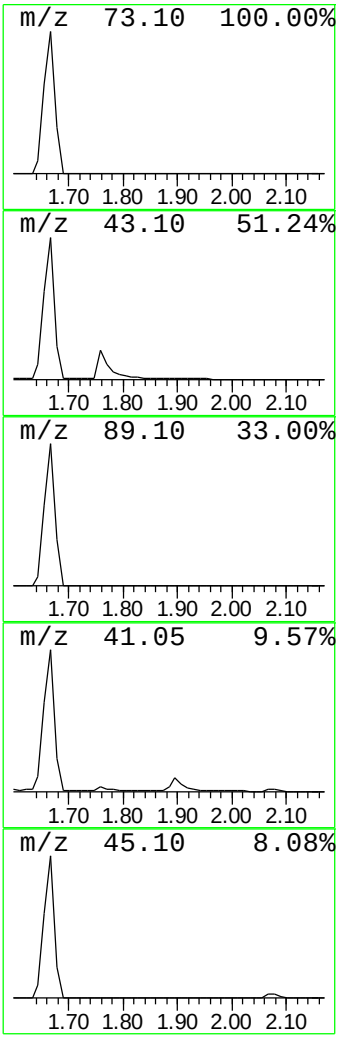
****

Peak Number 1 unknown1.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	178.38 ng	4834060	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

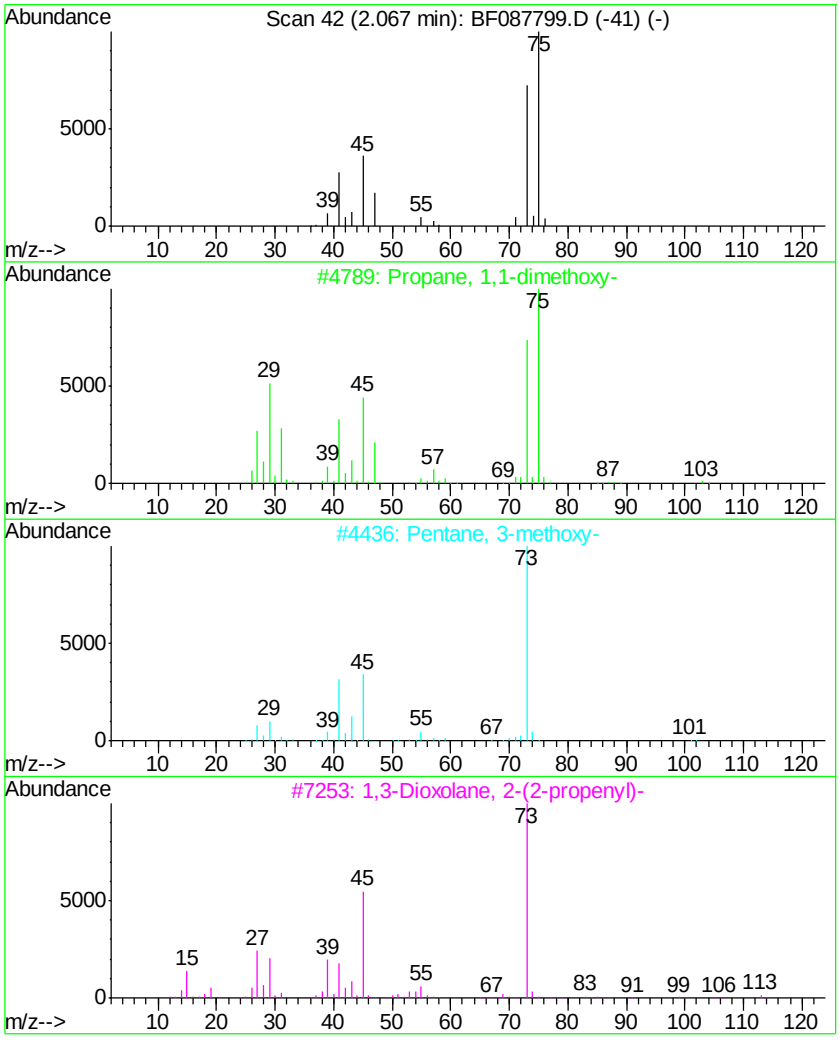
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

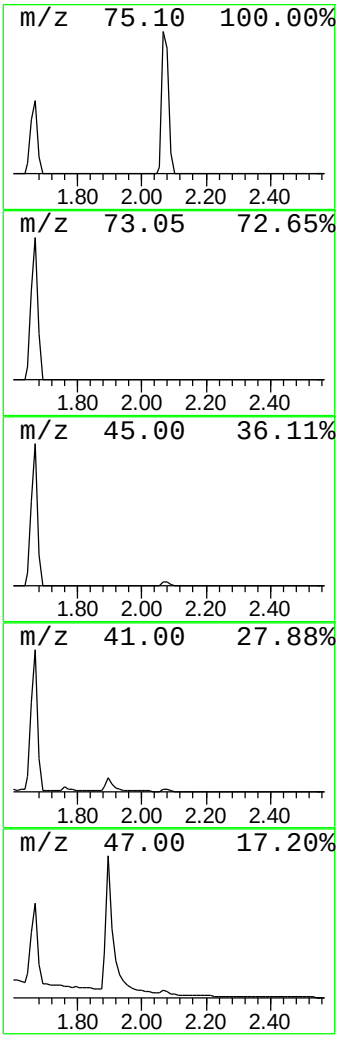
****

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	7.28 ng	197248	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
3	1,3-Dioxolane, 2-(2-propenyl)-	114	C6H10O2	038653-49-5	9
4	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
5	Glycine	75	C2H5NO2	000056-40-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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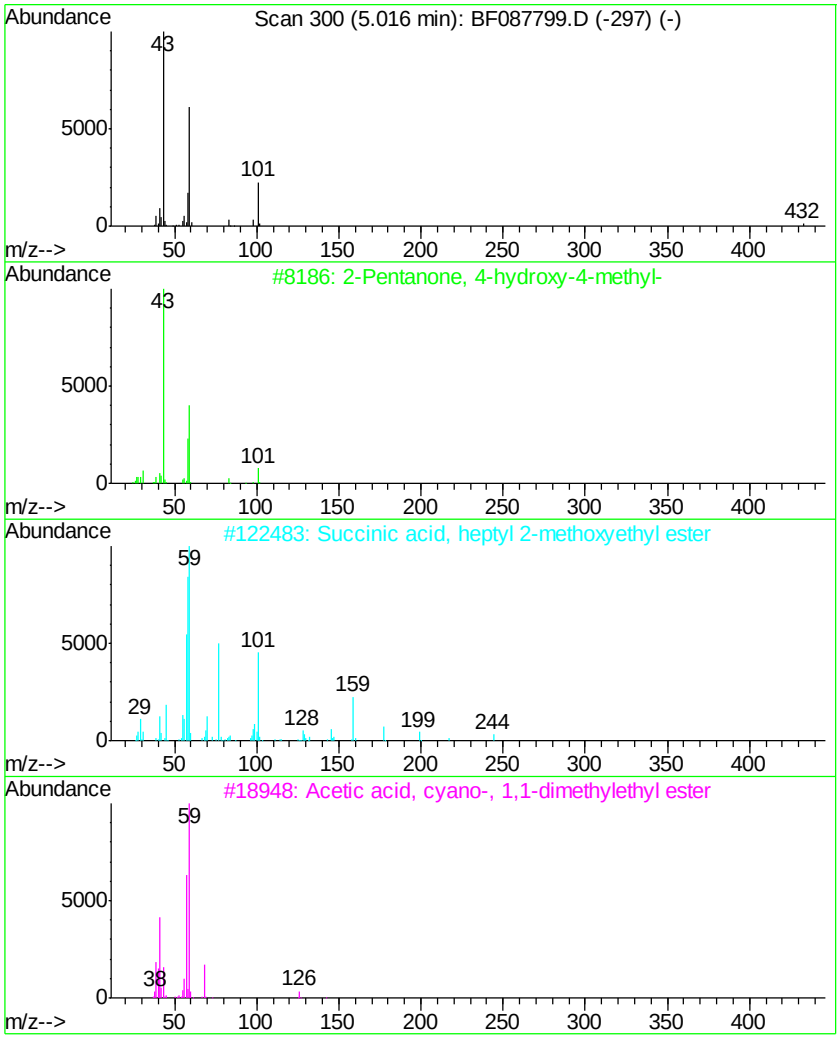
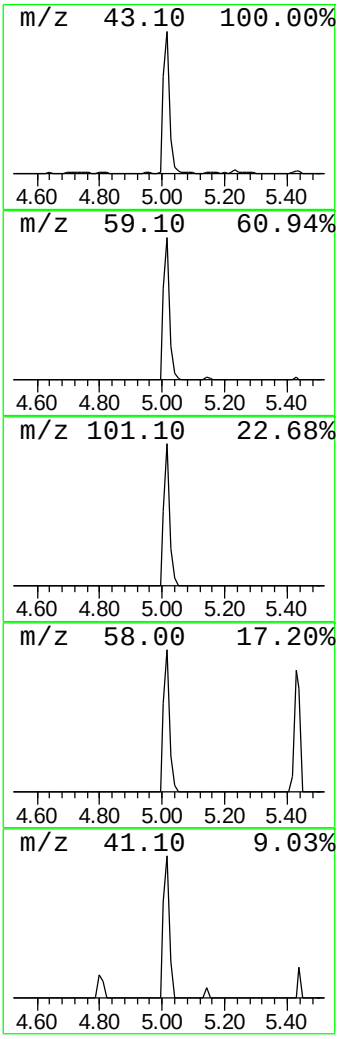
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	6.25 ng	169412	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33
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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087799.D
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Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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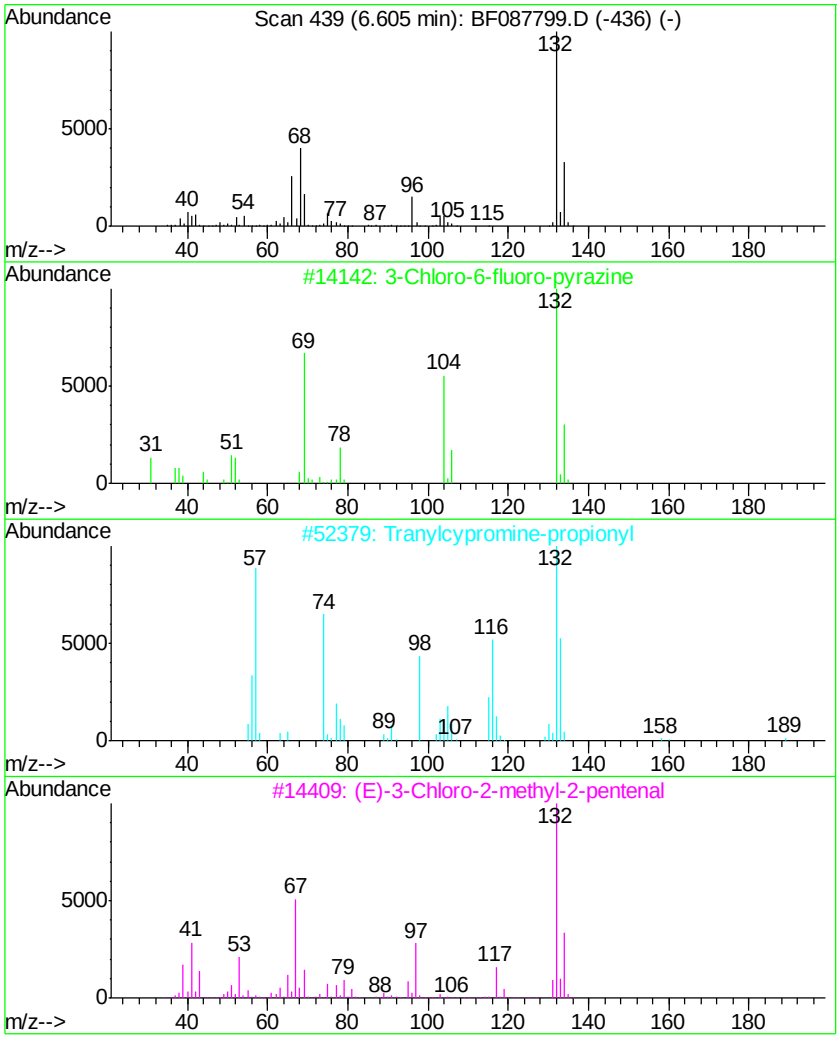
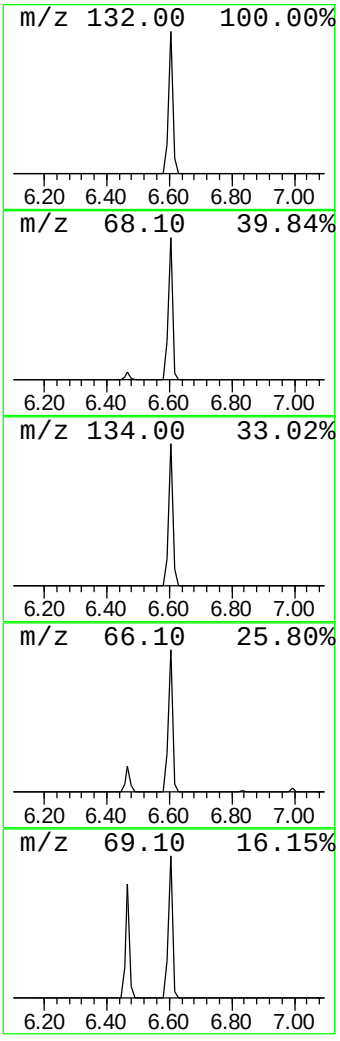
Peak Number 6 unknown6.60 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	61.37 ng	1663000	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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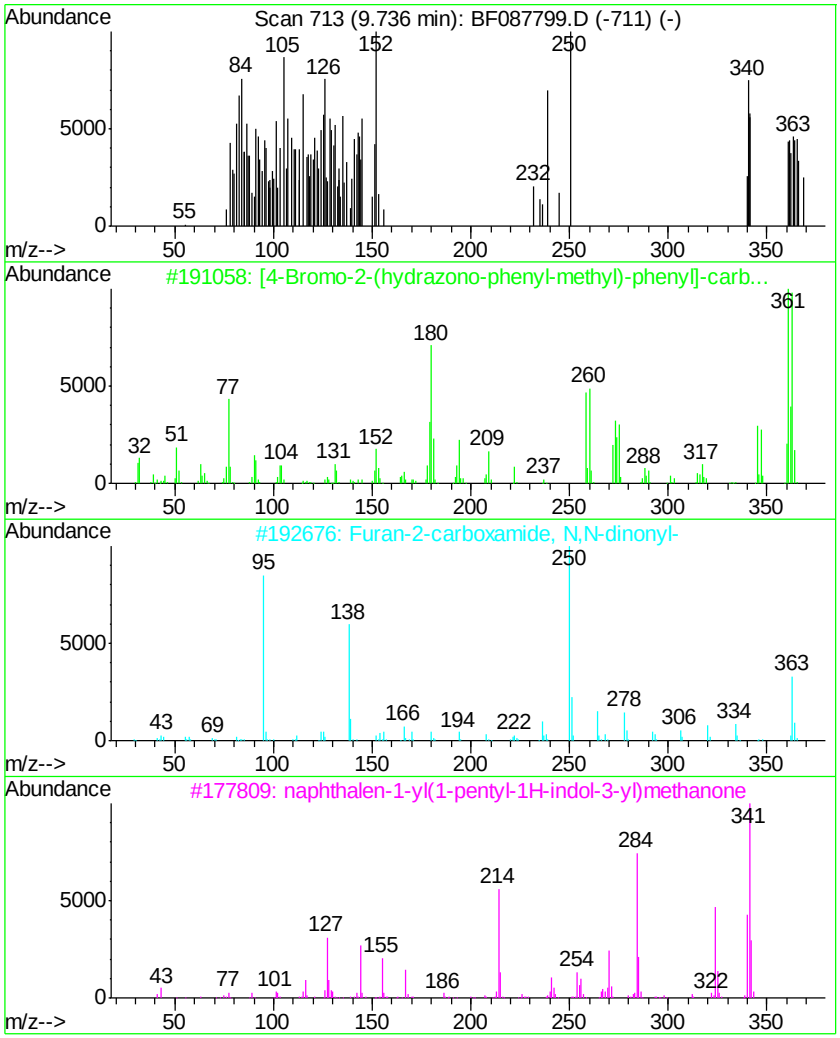
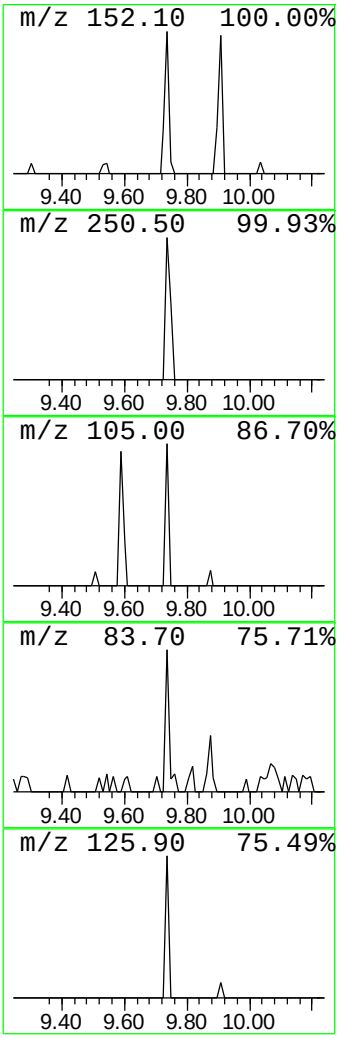
****

Peak Number 8 unknown9.74 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	3.13 ng	142426	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[4-Bromo-2-(hydrazono-phenyl-met...	361	C16H16BrN3O2	1000318-37-6	25
2	Furan-2-carboxamide, N,N-dinonyl-	363	C23H41NO2	1000308-21-0	10
3	naphthalen-1-yl(1-pentyl-1H-indo...	341	C24H23NO	209414-07-3	9
4	Carbamic acid, N-(3-chloro-4-met...	341	C18H28ClNO3	299202-69-0	9
5	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	9





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ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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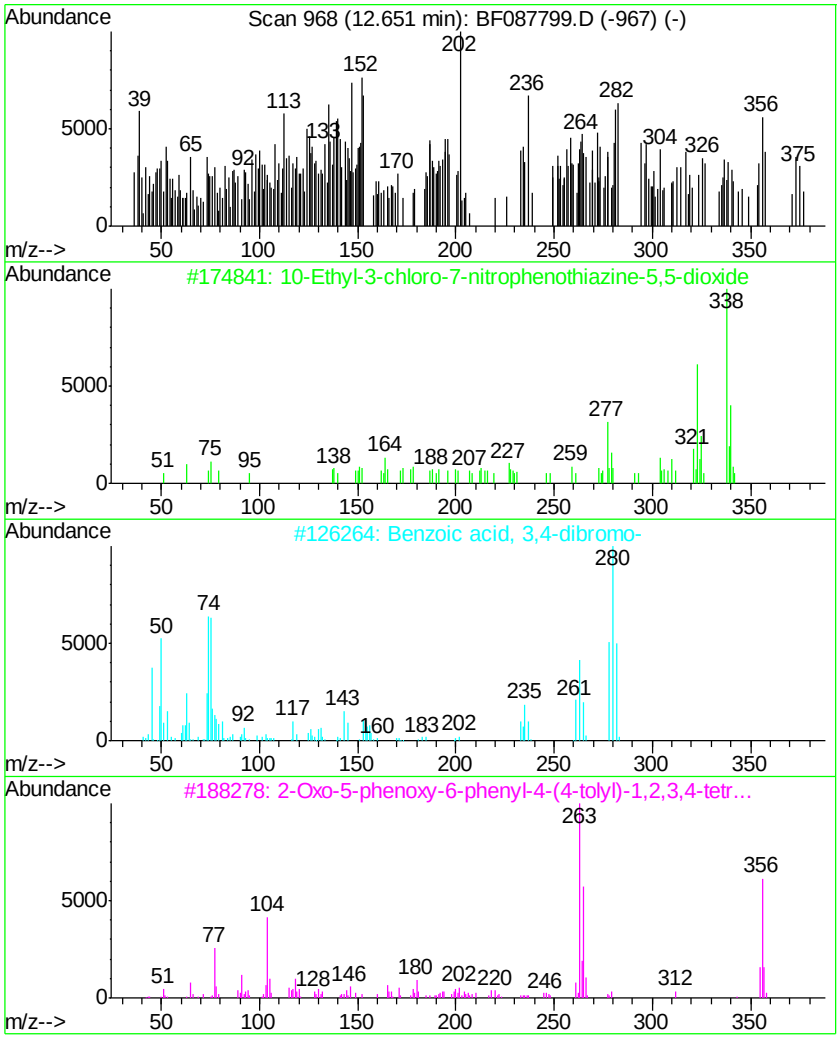
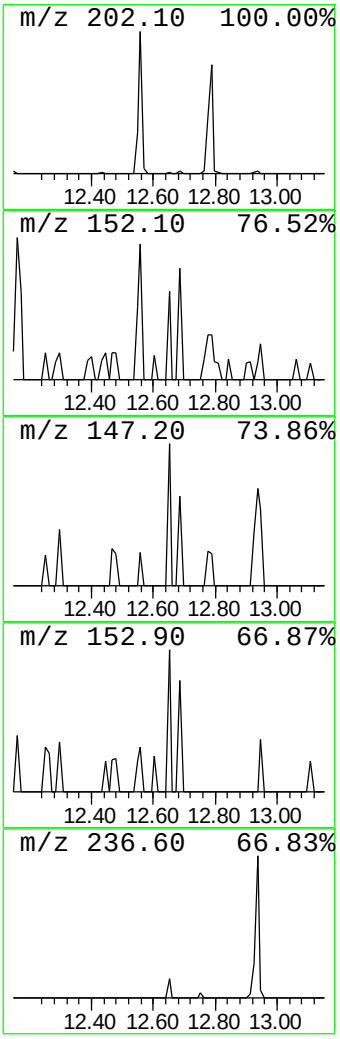
Peak Number 9 unknown12.65 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.09 ng	120173	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Ethyl-3-chloro-7-nitrophenoth...	338	C14H11ClN2O4S	024953-29-5	14
2	Benzoic acid, 3,4-dibromo-	278	C7H4Br2O2	000619-03-4	10
3	2-Oxo-5-phenoxy-6-phenyl-4-(4-to...	356	C23H20N2O2	1000070-60-3	10
4	Dimethoxymethyl-hydroxy-triphenyl...	354	C21H23O3P	1000132-00-1	9
5	1-[4-Chlorophenyl]-3-[3,5-dichlo...	310	C15H9Cl3O	1000250-94-3	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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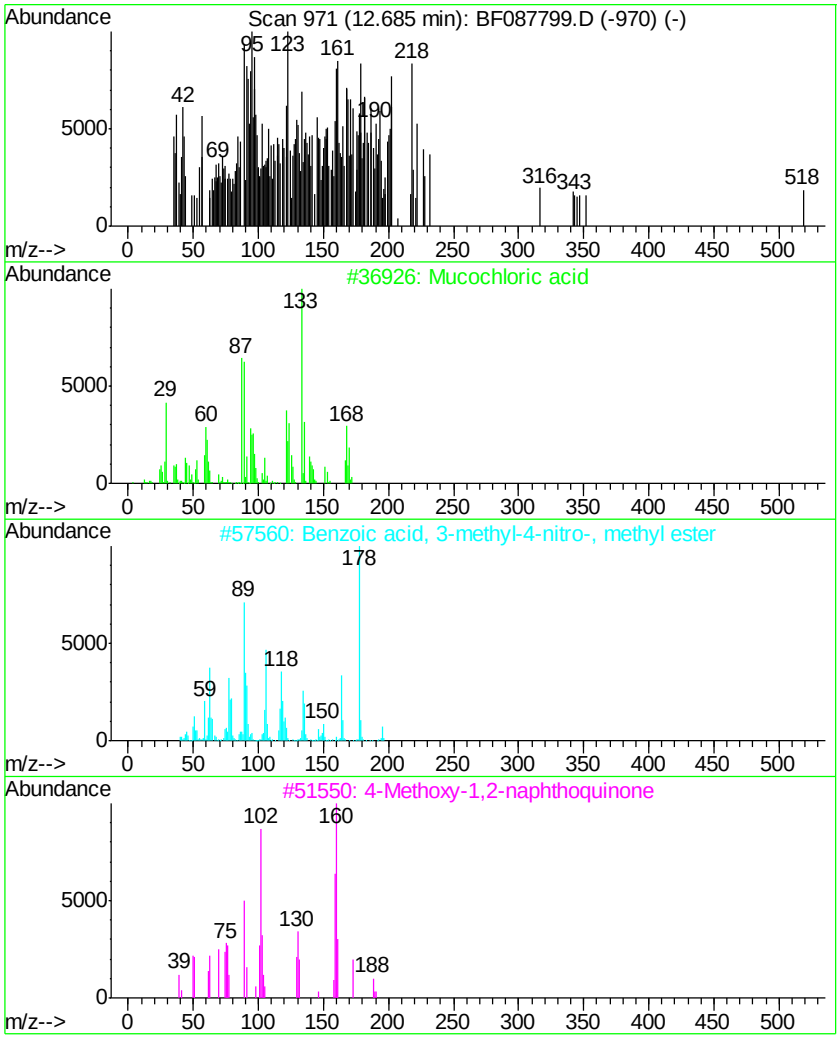
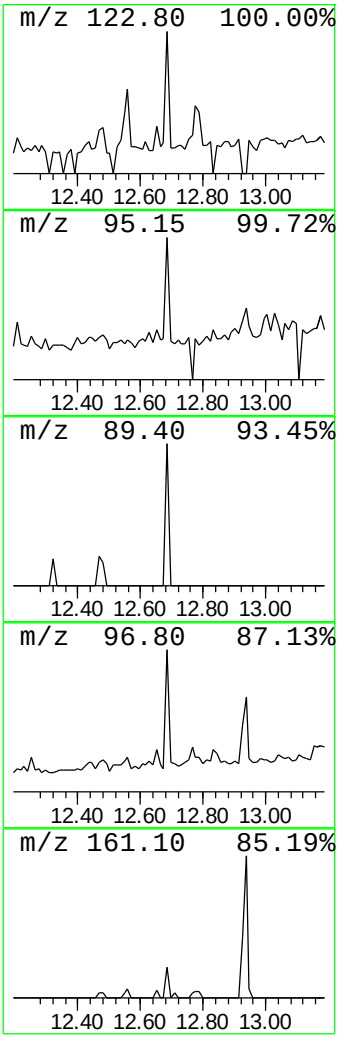
Peak Number 10 Mucochloric acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.69 ng	149751	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mucochloric acid	168	C4H2Cl2O3	000087-56-9	58
2	Benzoic acid, 3-methyl-4-nitro-,...	195	C9H9NO4	024078-21-5	50
3	4-Methoxy-1,2-naphthoquinone	188	C11H8O3	018916-57-9	49
4	5-[2-Chlorophenyl]tetraazole	180	C7H5ClN4	050907-46-5	45
5	Germacyclopent-3-ene, 1,1,3,4-te...	186	C8H16Ge	005764-66-9	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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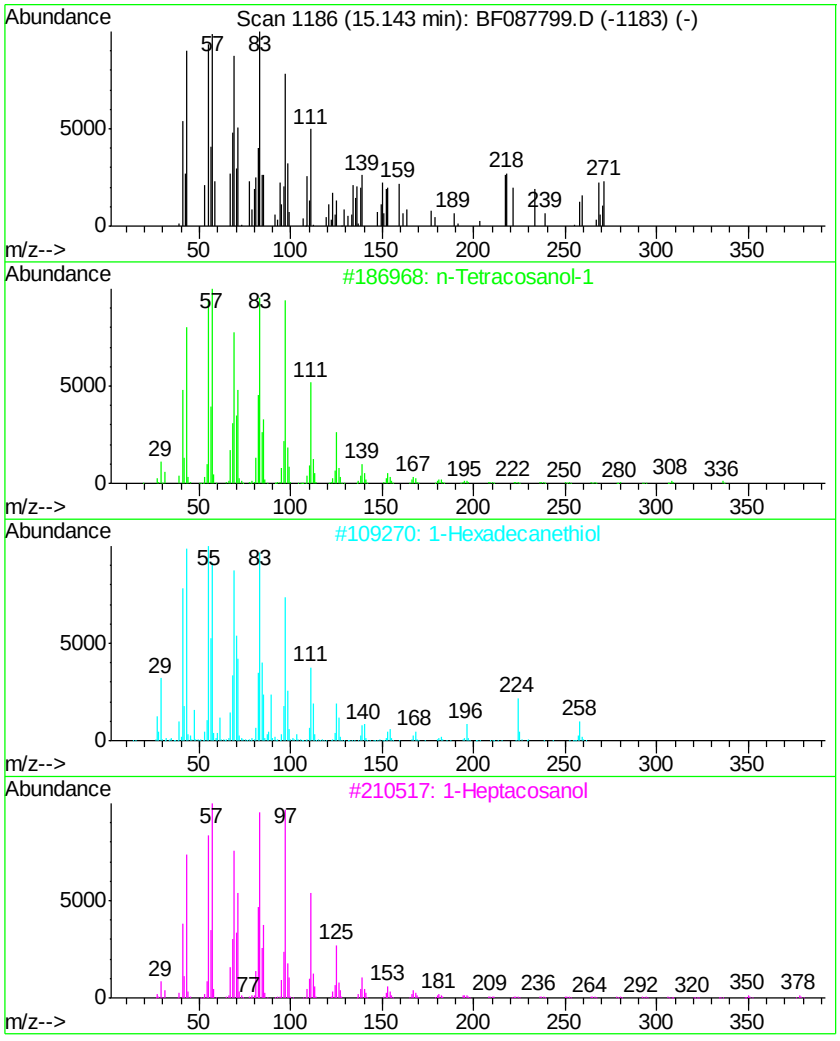
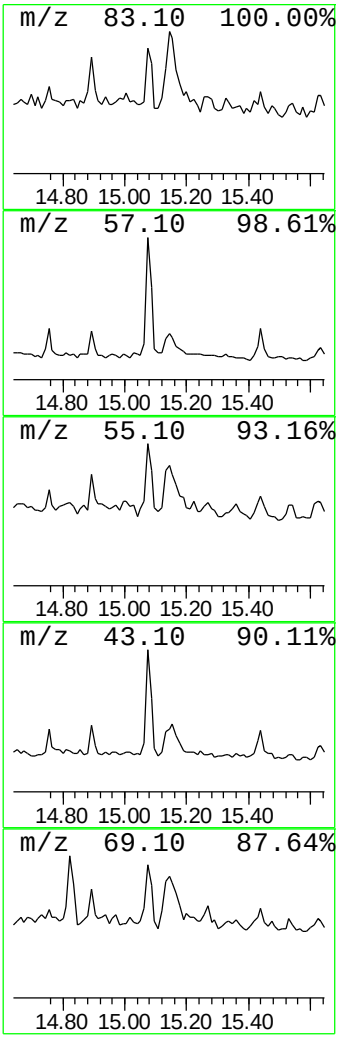
Peak Number 12 n-Tetracosanol-1 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.62 ng	90761	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
2	1-Hexadecanethiol	258	C16H34S	002917-26-2	68
3	1-Heptacosanol	396	C27H56O	002004-39-9	58
4	Behenic alcohol	326	C22H46O	000661-19-8	58
5	1-Heneicosanol	312	C21H44O	015594-90-8	58





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Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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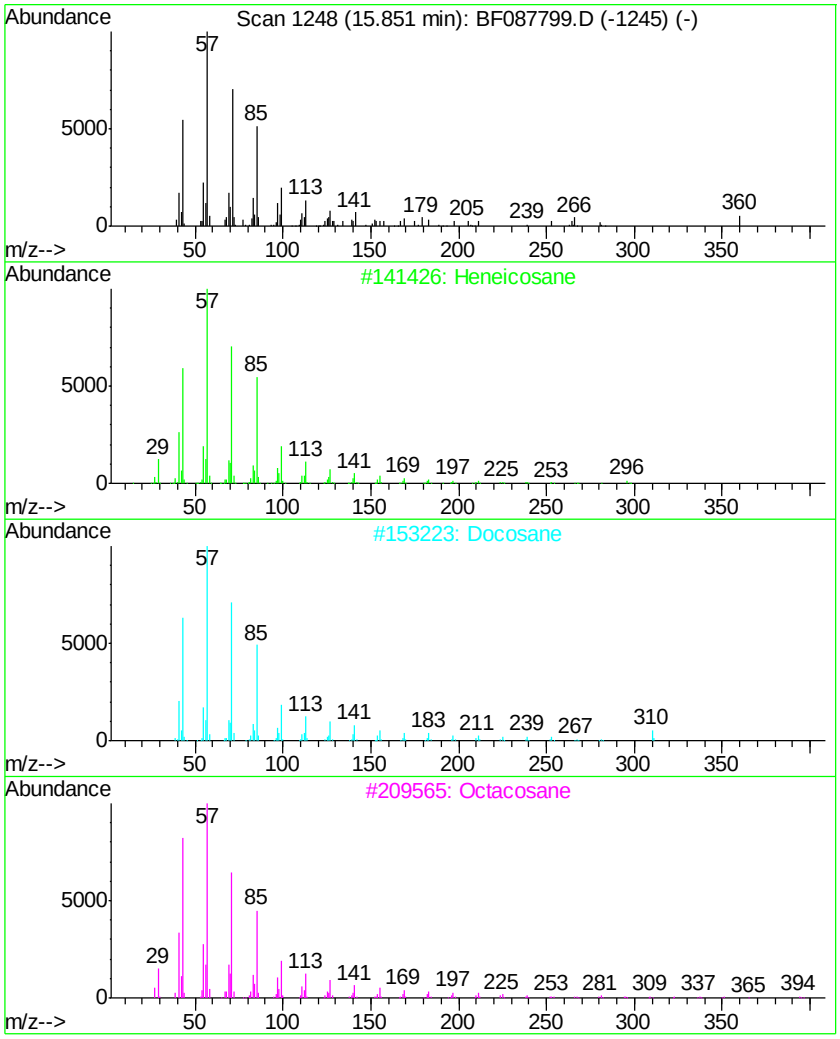
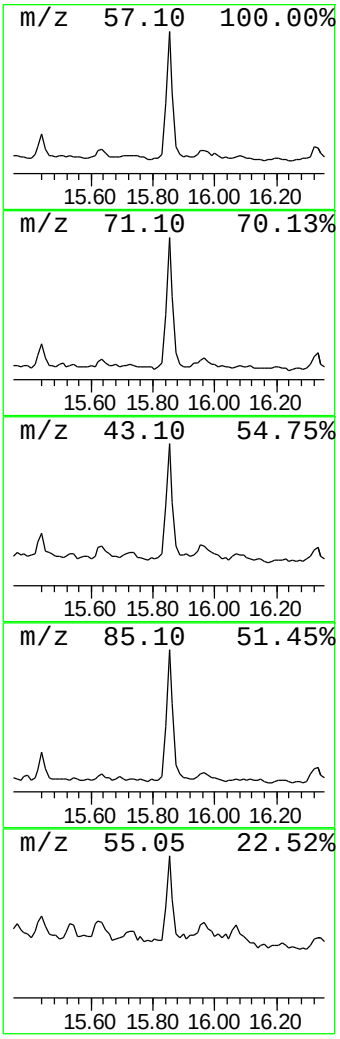
Peak Number 14 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	3.99 ng	137846	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Docosane	310	C22H46	000629-97-0	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Hexacosane	366	C26H54	000630-01-3	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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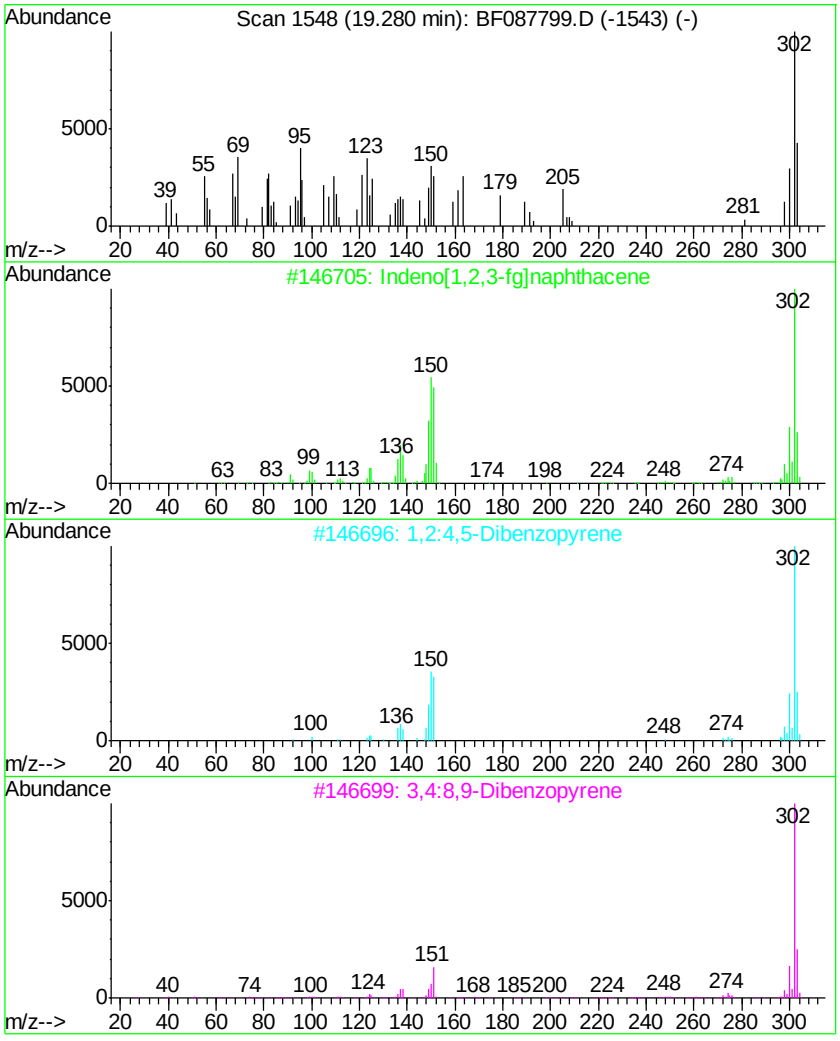
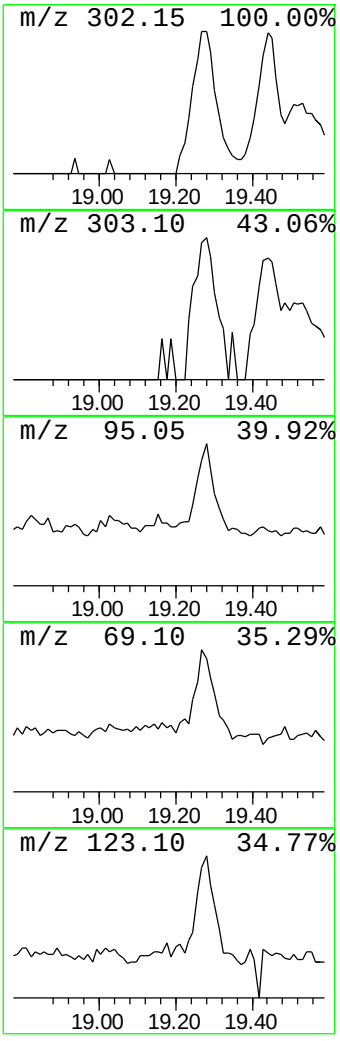
Peak Number 16 unknown19.28 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.28	3.28 ng	113447	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	43
2	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	43
3	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	38
4	Androstane-3,12,17-trione, (5.al...	302	C19H26O3	004171-01-1	35
5	Androst-4-ene-3,17-dione, 11-hyd...	302	C19H26O3	000382-44-5	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060716\
Data File : BF087799.D
Acq On : 7 Jun 2016 21:50
Operator : UM/SJ
Sample : H3379-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
unknown1.67	1.67	178.4	ng	4834060	1	6.83	541990	20.0
Propane, 1,1-dime...	2.07	7.3	ng	197248	1	6.83	541990	20.0
2-Pentanone, 4-hy...	5.02	6.3	ng	169412	1	6.83	541990	20.0
unknown6.60	6.60	61.4	ng	1663000	1	6.83	541990	20.0
unknown9.74	9.74	3.1	ng	142426	3	9.87	909128	20.0
unknown12.65	12.65	2.1	ng	120173	4	11.35	1149400	20.0
Mucochloric acid	12.69	2.7	ng	149751	5	13.98	1113980	20.0
n-Tetracosanol-1	15.14	2.6	ng	90761	6	15.39	691538	20.0
Heneicosane	15.85	4.0	ng	137846	6	15.39	691538	20.0
unknown19.28	19.28	3.3	ng	113447	6	15.39	691538	20.0