LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082317\
Data File : BF097995.D
Acq On : 23 Aug 2017 13:52
Operator : SJ/JU
Sample : I4901-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BE1-1-3-COMP

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-BF081517.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	2.116	3	5	18	rVB2	24668	53844	1.29%	0.153%
2	3.134	175	178	190	rBV	88167	159191	3.82%	0.451%
3	4.946	483	486	497	rVB	290214	459435	11.04%	1.302%
4	5.357	549	556	559	rBV	3335375	3942620	94.72%	11.172%
5	6.381	723	730	733	rBV	3494785	4162384	100.00%	11.795%
6	6.510	747	752	755	rBV	3572431	3902337	93.75%	11.058%
7	6.740	787	791	794	rBV	1139802	952747	22.89%	2.700%
8	6.898	813	818	821	rBV	3020908	2970415	71.36%	8.417%
9	7.304	881	887	890	rBV	2429219	2561839	61.55%	7.259%
10	8.022	1004	1009	1012	rBV	1409663	1276322	30.66%	3.617%
11	9.098	1186	1192	1195	rBV	3846173	4004177	96.20%	11.346%
12	9.492	1254	1259	1262	rBV	512275	422562	10.15%	1.197%
13	9.775	1301	1307	1310	rBV	1424051	1357282	32.61%	3.846%
14	10.557	1435	1440	1444	rBV	1692538	1756739	42.21%	4.978%
15	10.680	1458	1461	1468	rBV	70078	76826	1.85%	0.218%
16	11.128	1534	1537	1540	rBV	51837	45398	1.09%	0.129%
17	11.251	1554	1558	1561	rBV	1387324	1368305	32.87%	3.877%
18	11.275	1561	1562	1565	rVV	104115	61230	1.47%	0.174%
19	12.463	1755	1764	1767	rBV	128377	143851	3.46%	0.408%
20	12.669	1795	1799	1800	rBV2	100337	86936	2.09%	0.246%
21	12.686	1800	1802	1805	rVB	112526	93462	2.25%	0.265%
22	12.845	1823	1829	1832	rBV	3221990	3275381	78.69%	9.281%
23	13.321	1905	1910	1914	rBV	107815	106252	2.55%	0.301%
24	13.369	1915	1918	1921	rBV	51916	47557	1.14%	0.135%
25	13.739	1977	1981	1989	rVB2	161038	198520	4.77%	0.563%
26	13.880	2000	2005	2008	rBV	986852	1057205	25.40%	2.996%
27	14.892	2174	2177	2180	rBV2	37979	49830	1.20%	0.141%
28	15.298	2241	2246	2250	rBV	585189	697815	16.76%	1.977%

Sum of corrected areas: 35290462

LSC Report - Integrated Chromatogram

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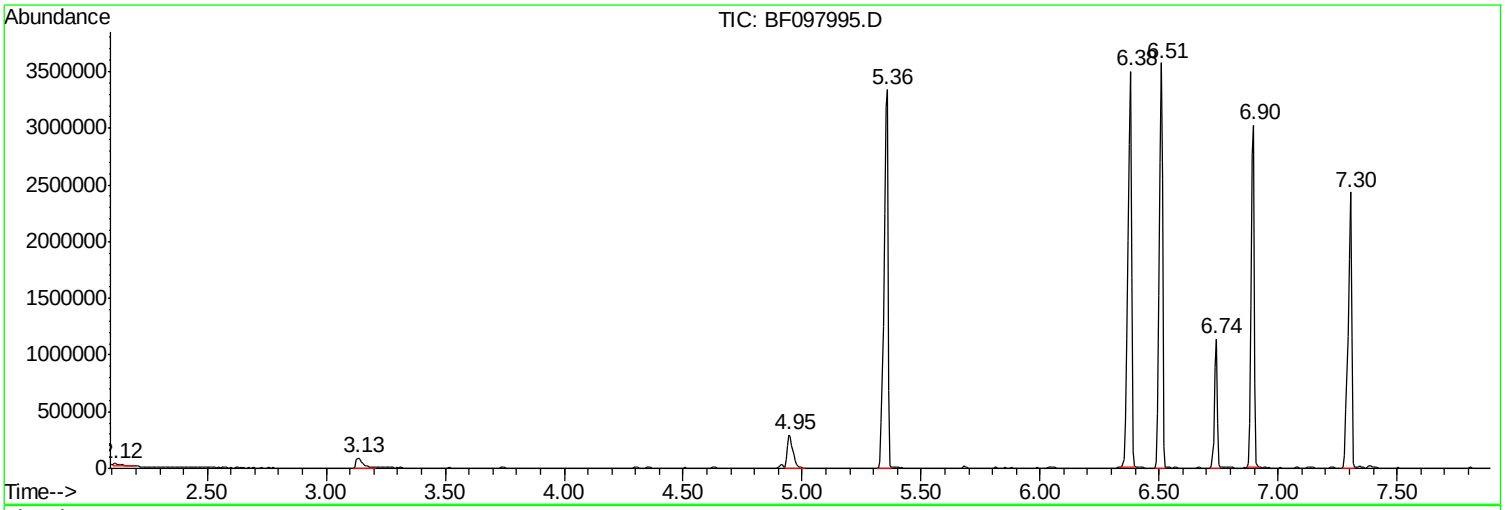
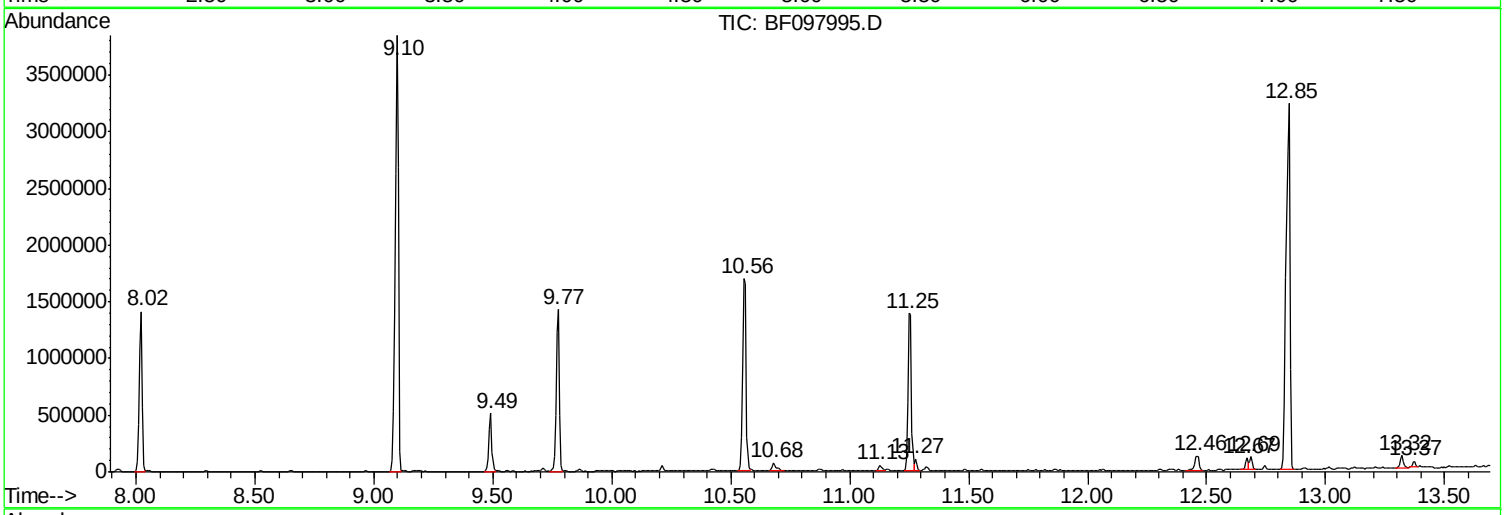
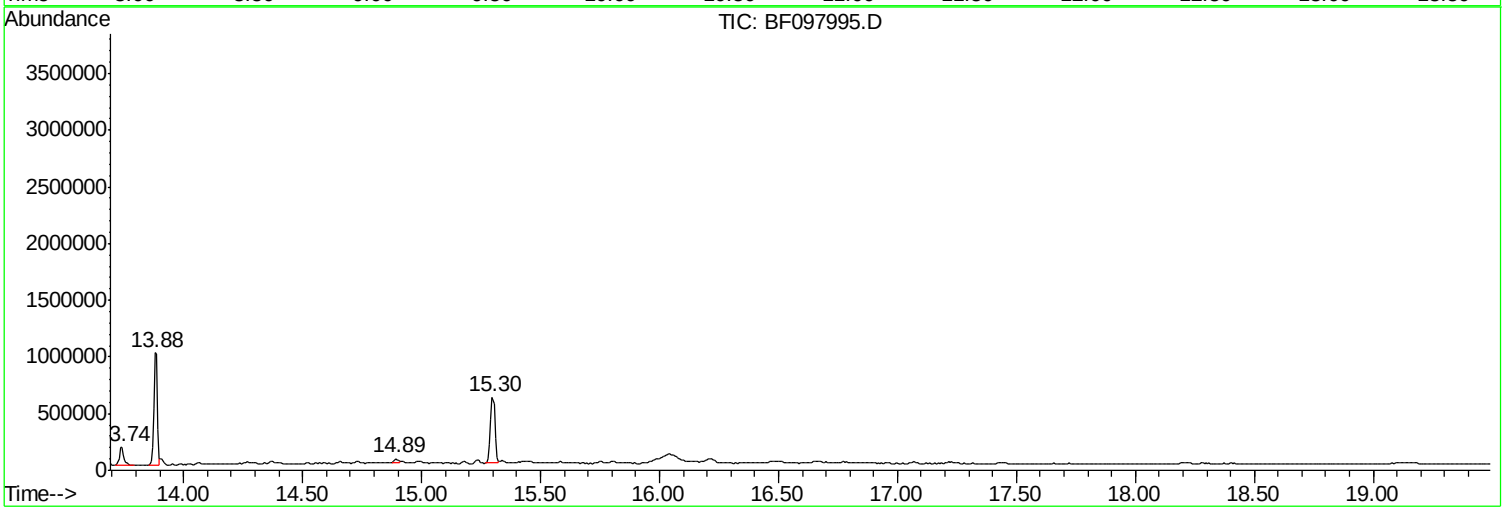
ClientSampleId :
TEC-BE1-1-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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

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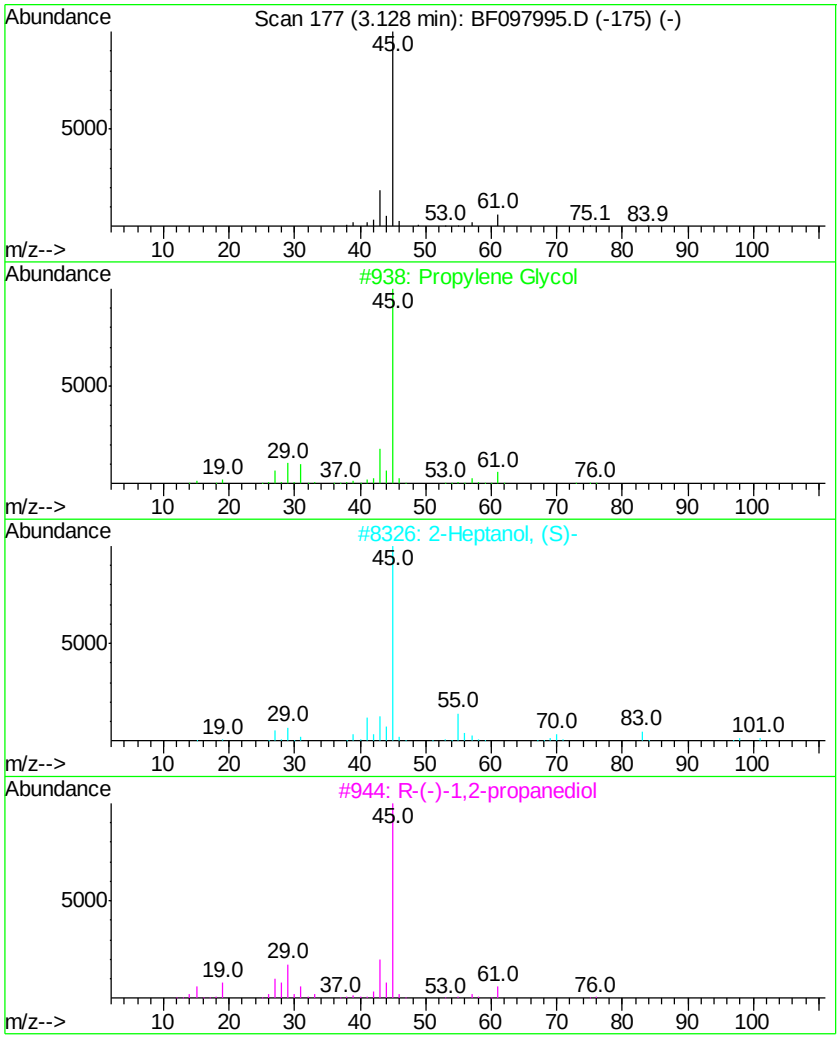
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

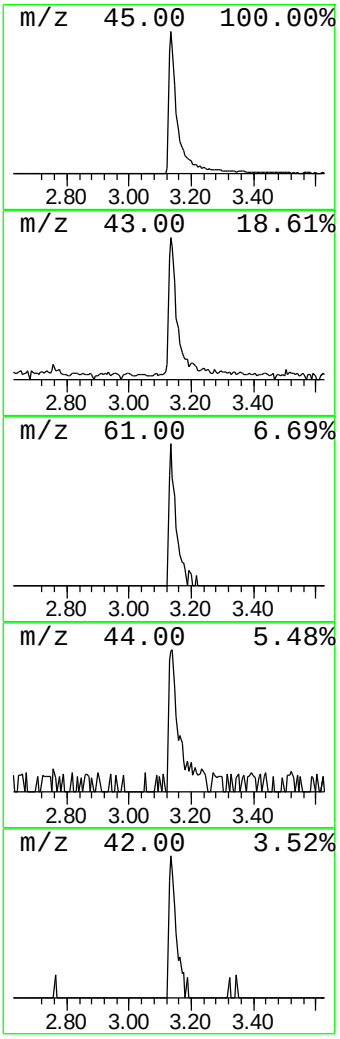
****

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	3.34 ng	159191	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	64
2	2-Heptanol, (S)-	116	C7H16O	006033-23-4	9
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9





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Misc :
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Instrument :
BNA_F
ClientSampleId :
TEC-BE1-1-3-COMP

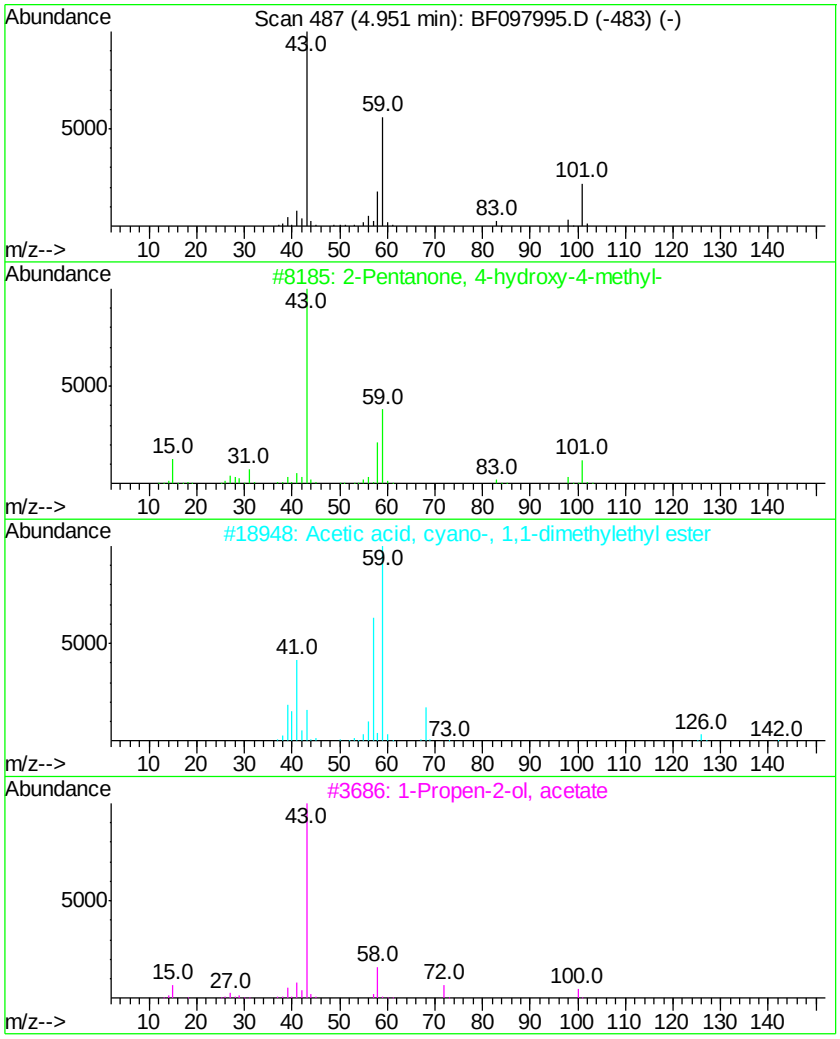
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

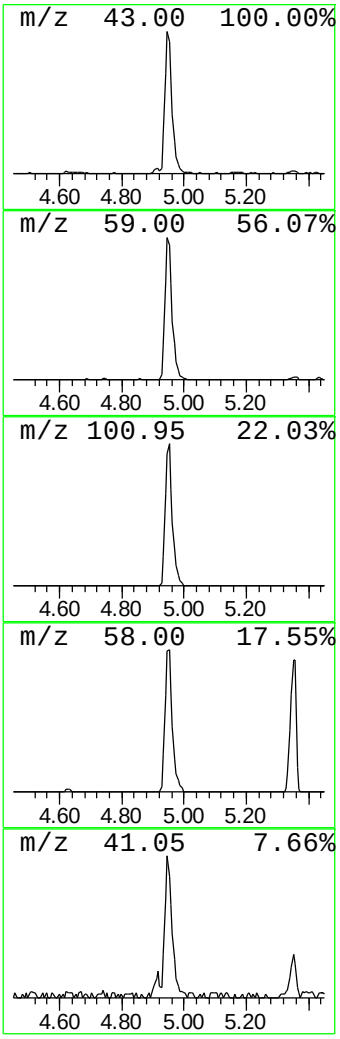
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	9.64 ng	459435	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument :
BNA_F
ClientSampleId :
TEC-BE1-1-3-COMP

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TIC Library : C:\DATABASE\NIST11.L
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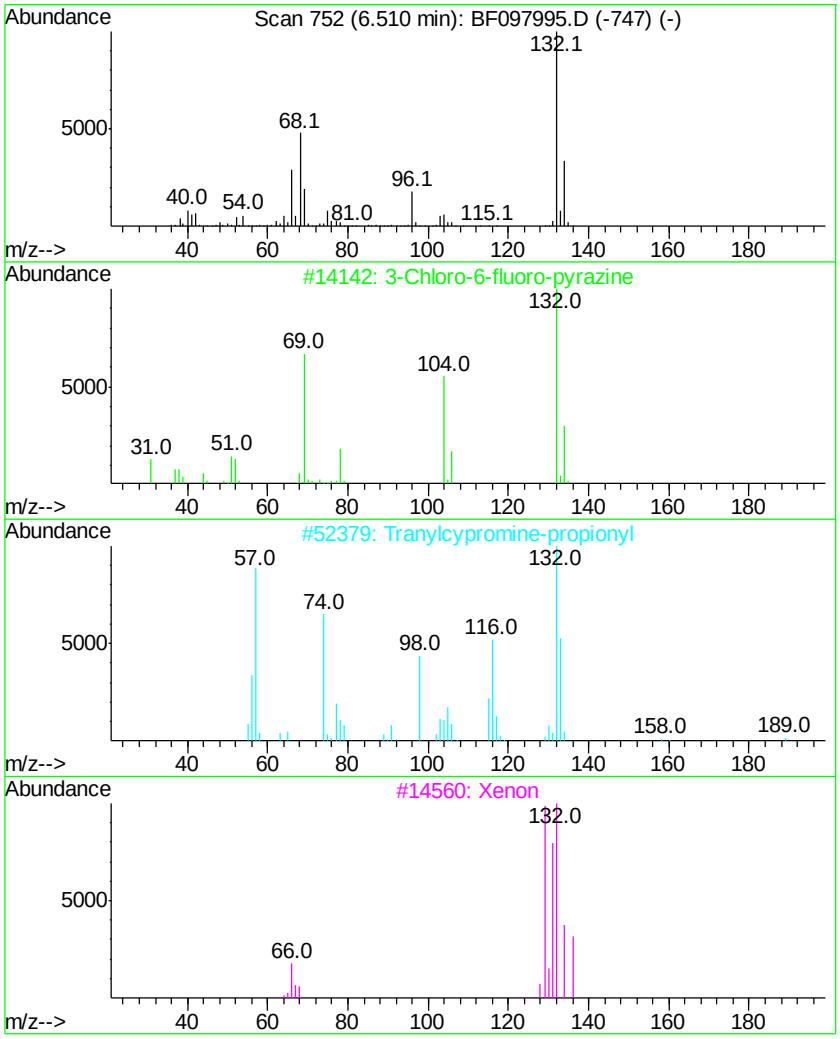
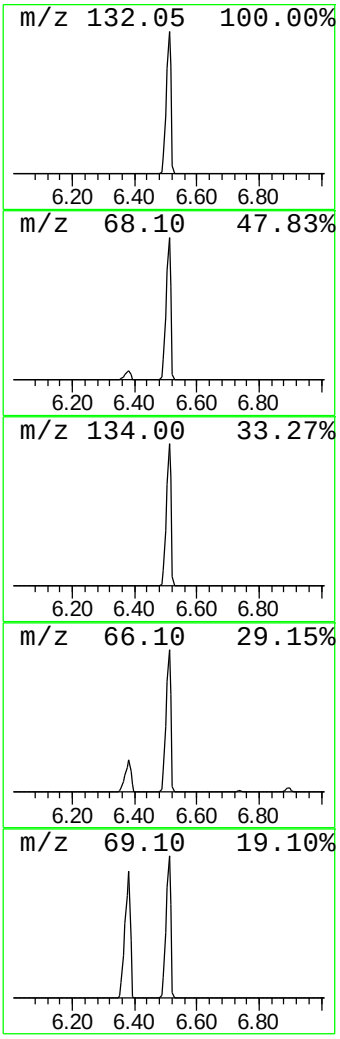
****

Peak Number 3 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	81.92 ng	3902340	1,4-Dichlorobenzene-d4	6.74

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	Xenon	132	Xe	007440-63-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument :
BNA_F
ClientSampleId :
TEC-BE1-1-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
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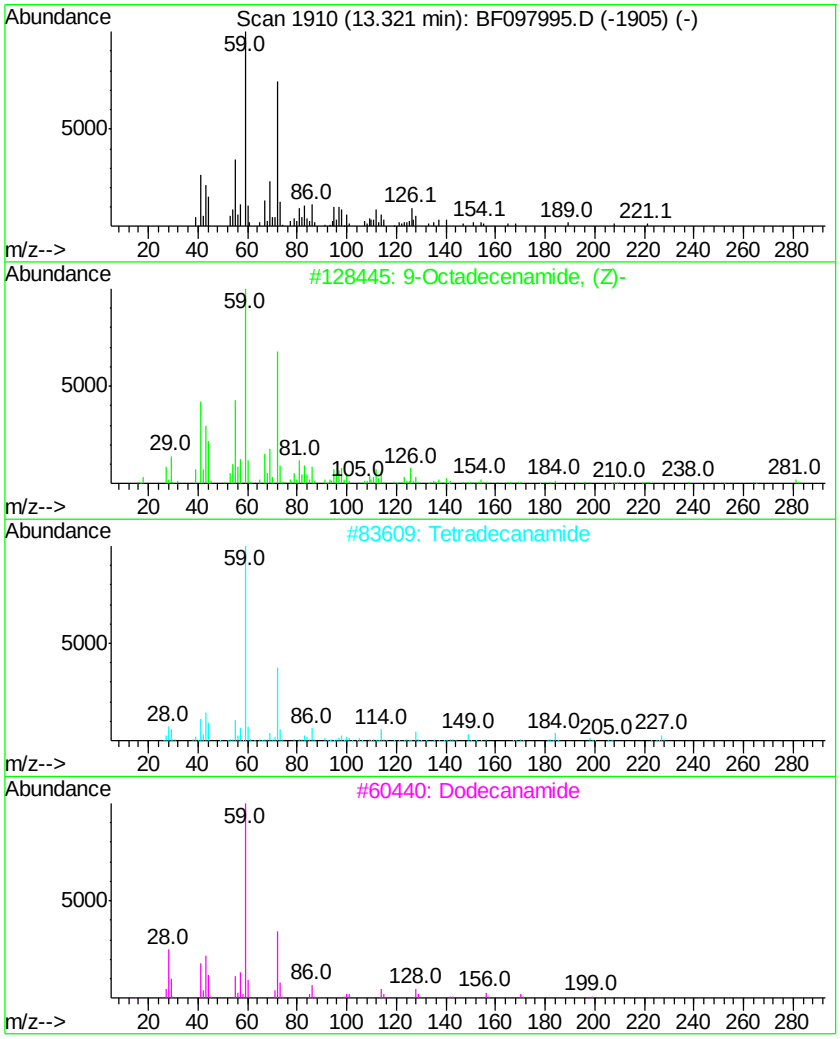
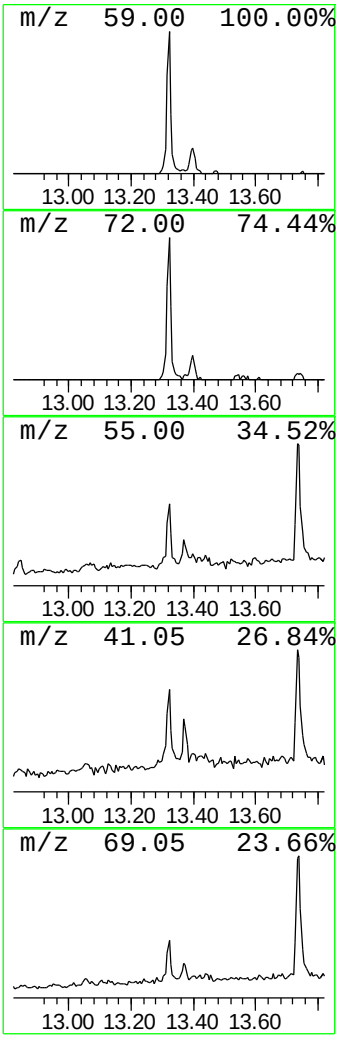
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	2.01 ng	106252	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	47
3	Dodecanamide	199	C12H25NO	001120-16-7	43
4	Octanamide	143	C8H17NO	000629-01-6	37
5	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	35





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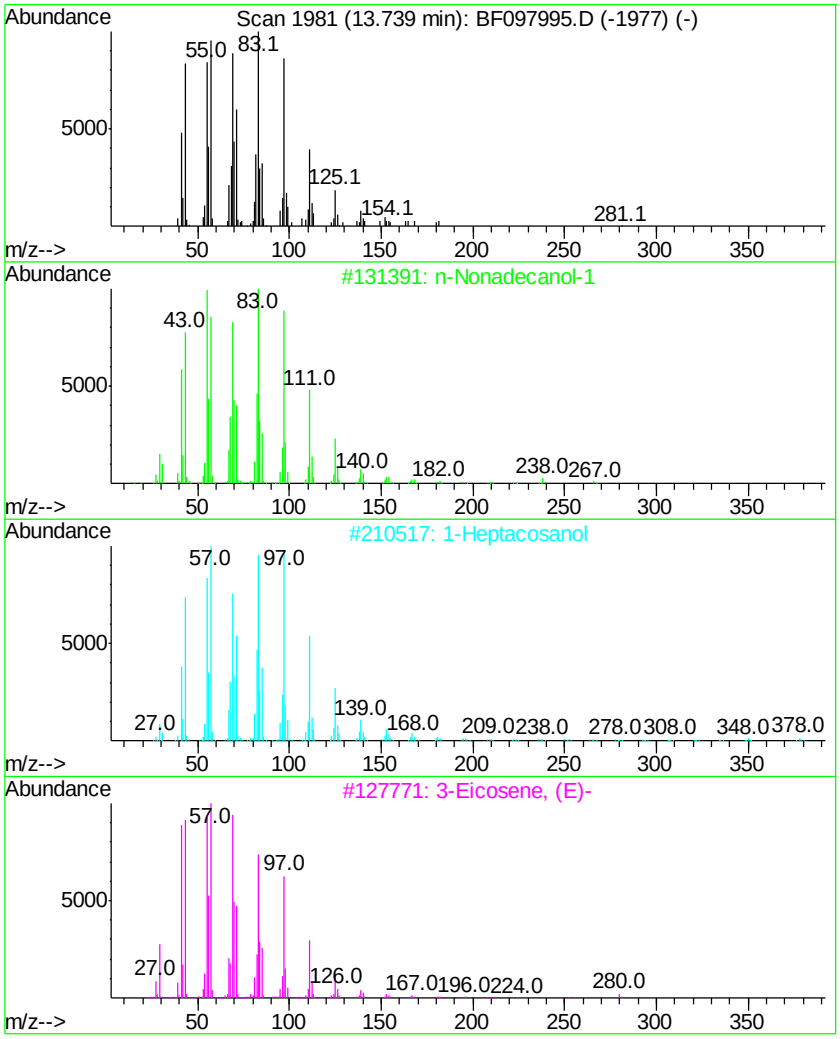
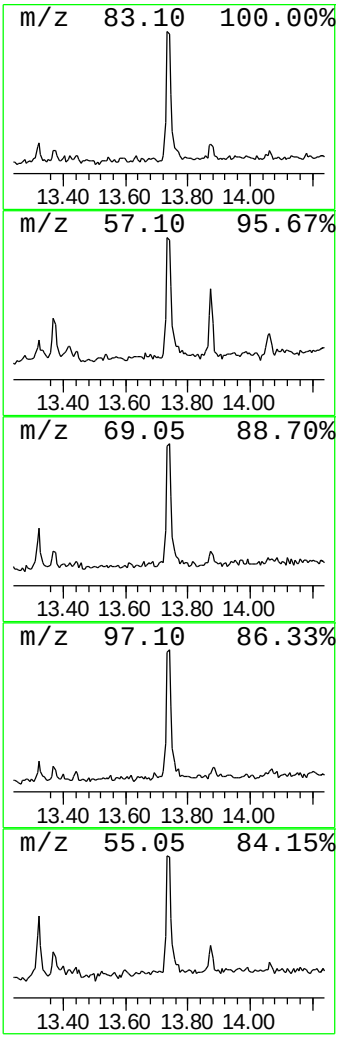
****

Peak Number 7 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.76 ng	198520	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	90





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Propylene Glycol	3.13	3.3	ng	159191	1	6.74	952747	20.0
2-Pentanone, 4-hy...	4.95	9.6	ng	459435	1	6.74	952747	20.0
unknown6.51	6.51	81.9	ng	3902340	1	6.74	952747	20.0
9-Octadecenamide,...	13.32	2.0	ng	106252	5	13.89	1057210	20.0
n-Nonadecanol-1	13.74	3.8	ng	198520	5	13.89	1057210	20.0