LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097174.D
Acq On : 29 Jul 2017 00:42
Operator : SJ/JU
Sample : I4456-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

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-BF072517.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	4.628	462	466	482	rBB	567220	844579	29.35%	3.601%
2	5.087	540	544	564	rBV	2198709	2423695	84.24%	10.334%
3	6.151	720	725	739	rBV	2574195	2877245	100.00%	12.268%
4	6.257	739	743	747	rBV	2504786	2457416	85.41%	10.478%
5	6.486	778	782	790	rBV	860248	738820	25.68%	3.150%
6	6.639	804	808	812	rBV	1820035	1827084	63.50%	7.790%
7	7.057	874	879	882	rBV	1761947	1666143	57.91%	7.104%
8	7.192	899	902	913	rVB	24765	30150	1.05%	0.129%
9	7.769	996	1000	1009	rBV	1112590	926750	32.21%	3.952%
10	8.845	1179	1183	1187	rBV	2017685	1747719	60.74%	7.452%
11	9.245	1247	1251	1254	rBV	353951	264060	9.18%	1.126%
12	9.516	1292	1297	1300	rVV	805340	772471	26.85%	3.294%
13	9.969	1371	1374	1377	rVB	40440	31295	1.09%	0.133%
14	10.298	1427	1430	1435	rBV	899769	783223	27.22%	3.340%
15	10.439	1450	1454	1466	rVB	60187	84600	2.94%	0.361%
16	10.886	1526	1530	1532	rBV	46871	43830	1.52%	0.187%
17	10.986	1542	1547	1549	rBV	655257	541071	18.81%	2.307%
18	11.010	1549	1551	1554	rVV	219265	172865	6.01%	0.737%
19	11.063	1556	1560	1565	rBV	56461	53040	1.84%	0.226%
20	11.304	1599	1601	1612	rVB3	21012	35193	1.22%	0.150%
21	11.486	1624	1632	1634	rBV	28321	40884	1.42%	0.174%
22	11.515	1634	1637	1639	rVV2	40498	45720	1.59%	0.195%
23	11.539	1639	1641	1644	rVV	77148	77474	2.69%	0.330%
24	11.598	1648	1651	1653	rBV	44531	41411	1.44%	0.177%
25	12.192	1748	1752	1756	rBV	437650	373771	12.99%	1.594%
26	12.415	1785	1790	1793	rBV	352550	364464	12.67%	1.554%
27	12.568	1813	1816	1823	rVB	1174391	1041280	36.19%	4.440%
28	12.639	1823	1828	1832	rBV2	25710	45672	1.59%	0.195%
29	12.745	1844	1846	1851	rVB2	50743	50996	1.77%	0.217%
30	12.815	1854	1858	1861	rBV2	35664	39629	1.38%	0.169%
31	12.851	1861	1864	1866	rBV	33299	30524	1.06%	0.130%
32	13.257	1931	1933	1937	rVB	33065	30547	1.06%	0.130%
33	13.362	1948	1951	1953	rBV	39365	37131	1.29%	0.158%
34	13.480	1966	1971	1977	rBV3	85478	132958	4.62%	0.567%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097174.D
Acq On : 29 Jul 2017 00:42
Operator : SJ/JU
Sample : I4456-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.609	1985	1993	1996	rBV2	748447	941684	32.73%	4.015%
36	13.633	1996	1997	2000	rVB	193928	149845	5.21%	0.639%
37	13.715	2008	2011	2016	rBV2	41066	43195	1.50%	0.184%
38	13.998	2055	2059	2063	rVB	38155	41432	1.44%	0.177%
39	14.115	2076	2079	2082	rBV3	26688	31783	1.10%	0.136%
40	14.374	2121	2123	2126	rBV4	25317	30661	1.07%	0.131%
41	14.468	2136	2139	2142	rVB2	32694	32128	1.12%	0.137%
42	14.604	2158	2162	2165	rBV	215046	302161	10.50%	1.288%
43	14.692	2174	2177	2183	rVB	58658	70756	2.46%	0.302%
44	14.856	2201	2205	2210	rVB	103330	132704	4.61%	0.566%
45	14.909	2210	2214	2218	rBV	141261	160263	5.57%	0.683%
46	14.962	2218	2223	2226	rBV	382933	459924	15.98%	1.961%
47	15.362	2288	2291	2296	rVB2	35668	43754	1.52%	0.187%
48	16.180	2425	2430	2437	rVB	68028	124074	4.31%	0.529%
49	16.250	2439	2442	2448	rVB6	30498	46101	1.60%	0.197%
50	16.321	2450	2454	2457	rBV5	24546	40382	1.40%	0.172%
51	16.415	2468	2470	2479	rVB10	20242	45232	1.57%	0.193%
52	16.539	2488	2491	2499	rVB	47160	82982	2.88%	0.354%

Sum of corrected areas: 23452771

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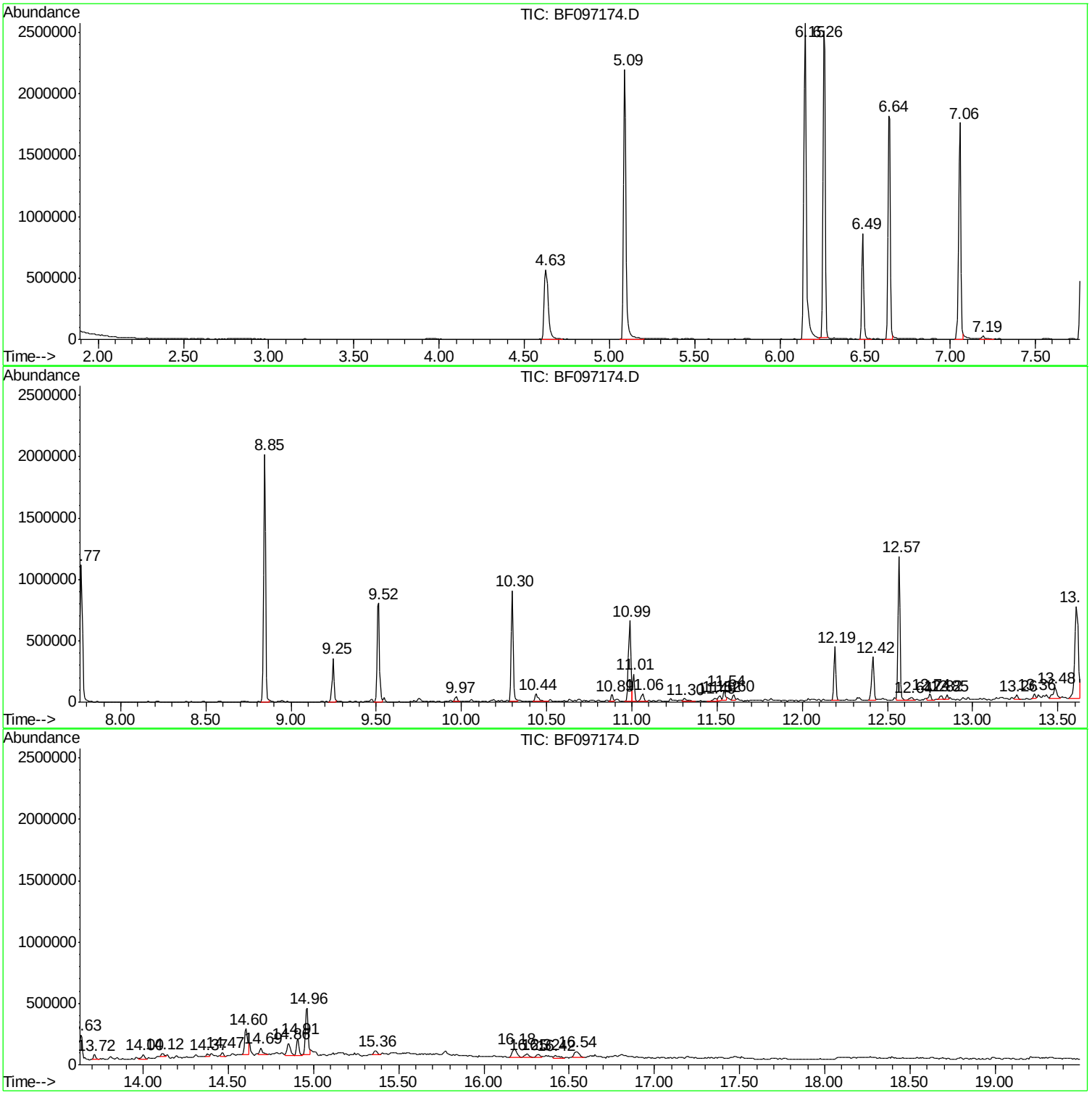
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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\BF072817\
Data File : BF097174.D
Acq On : 29 Jul 2017 00:42
Operator : SJ/JU
Sample : I4456-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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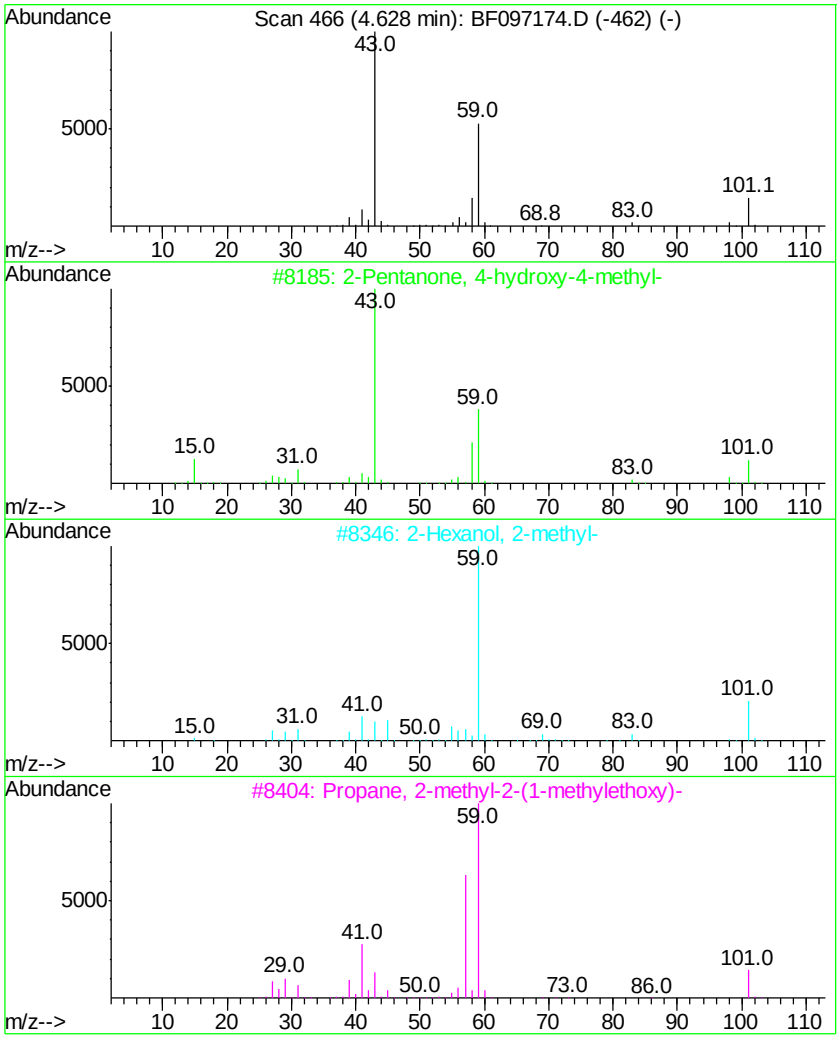
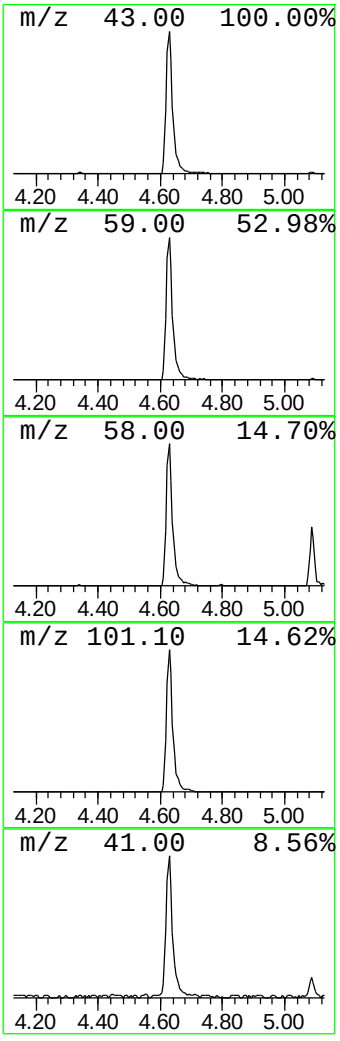
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	22.86 ng	844579	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097174.D
Acq On : 29 Jul 2017 00:42
Operator : SJ/JU
Sample : I4456-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

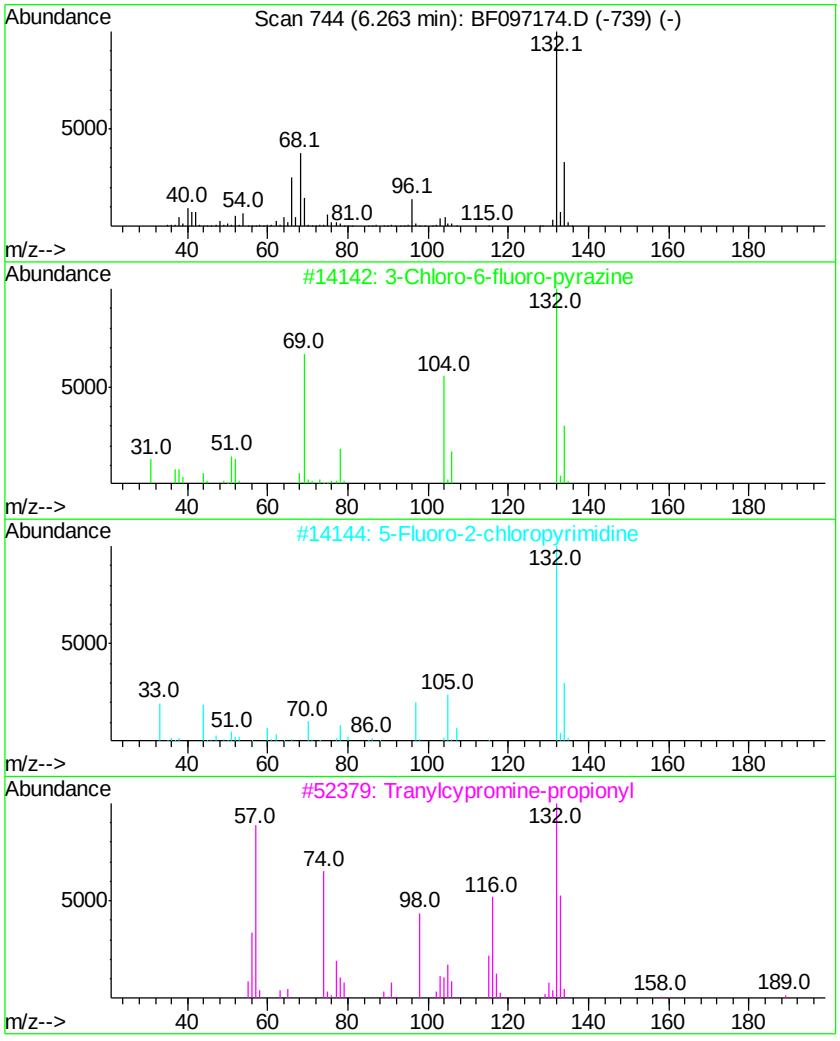
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

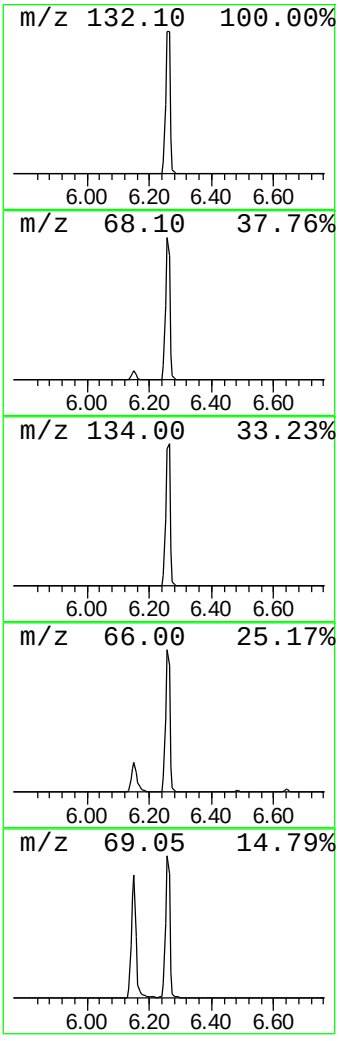
****

Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	66.52 ng	2457420	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Acq On : 29 Jul 2017 00:42
Operator : SJ/JU
Sample : I4456-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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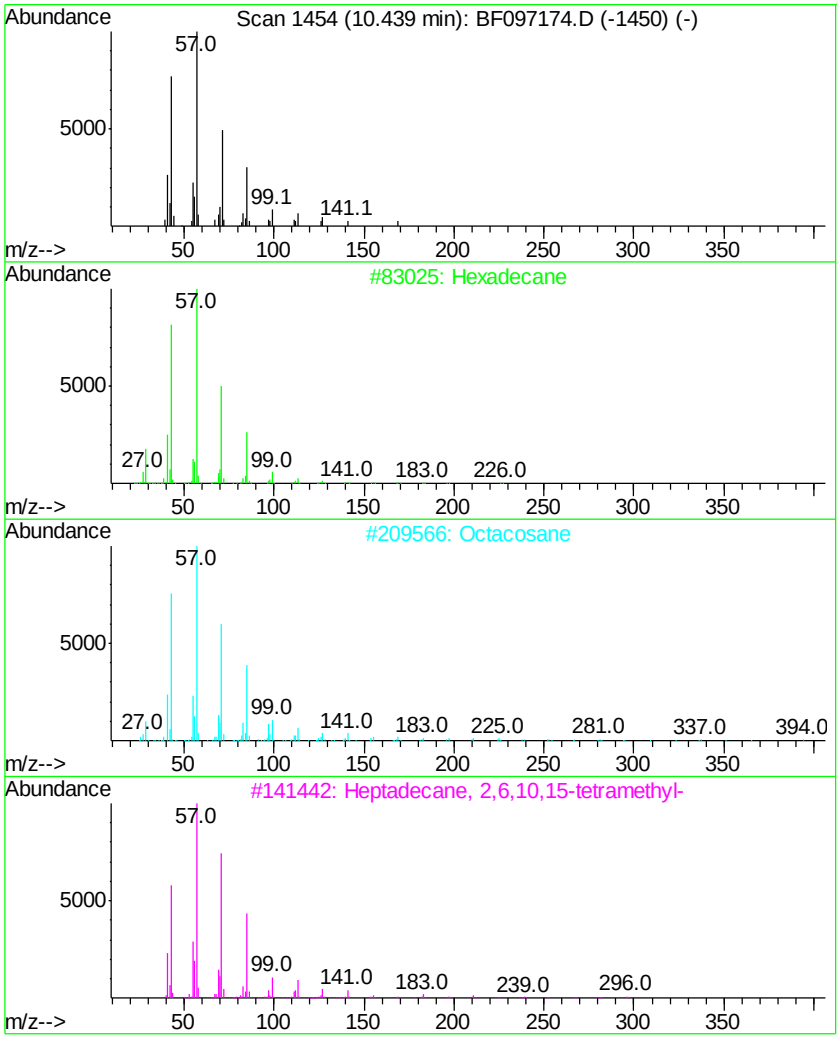
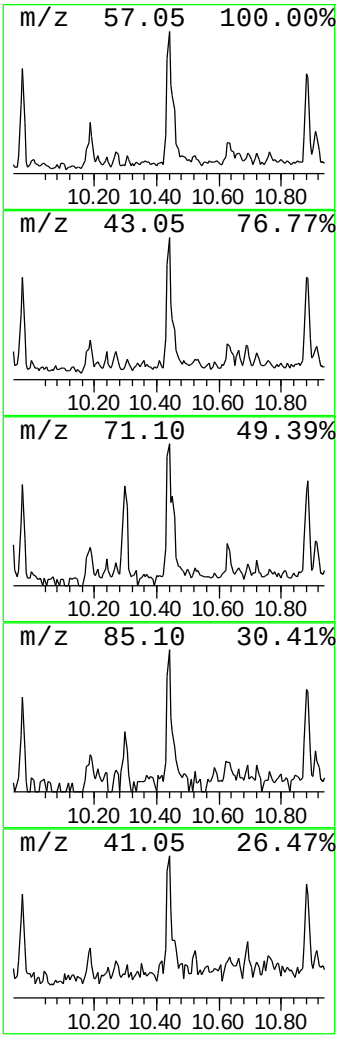
Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	3.13 ng	84600	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4	Hexacosane	366	C26H54	000630-01-3	86
5	Heptacosane	380	C27H56	000593-49-7	86





Library Search Compound Report

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Sample : I4456-07
Misc :
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Instrument : BNA_F
ClientSampleId : TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

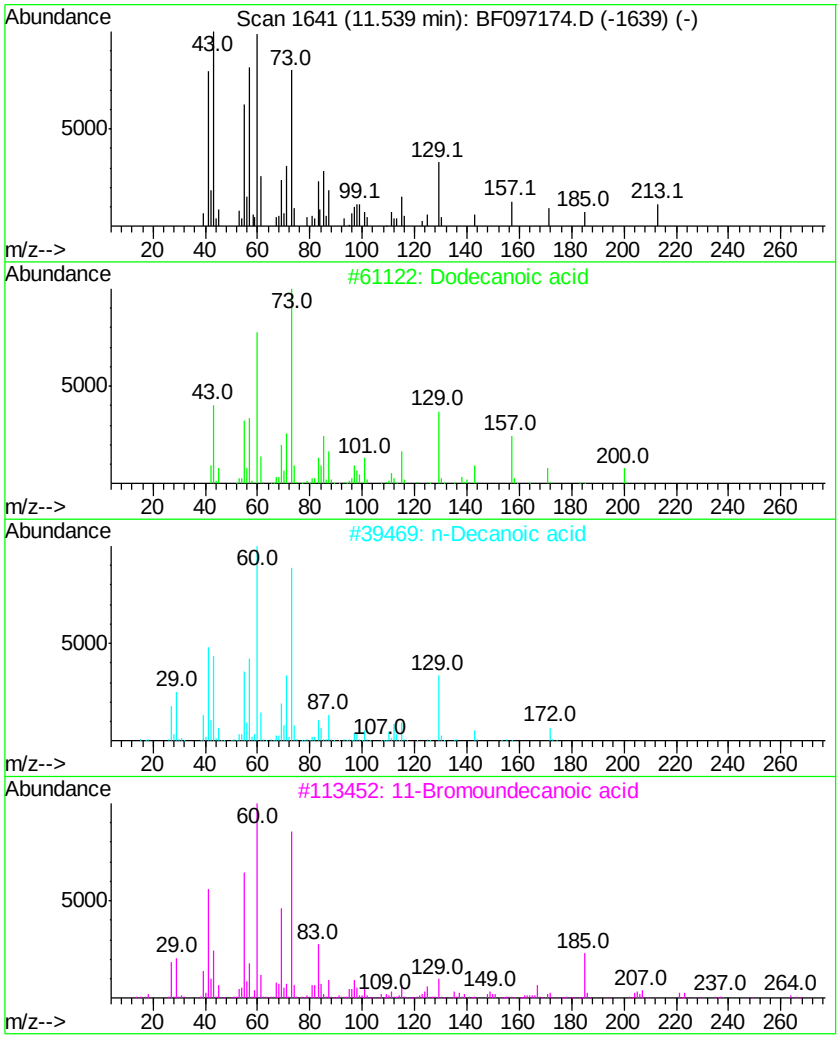
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

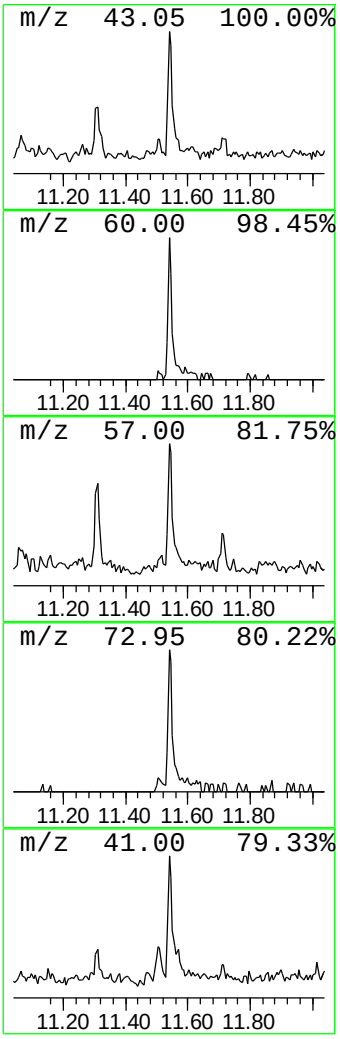
****

Peak Number 5 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.86 ng	77474	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	53
2	n-Decanoic acid	172	C10H20O2	000334-48-5	50
3	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	43
4	Undecanoic acid	186	C11H22O2	000112-37-8	40
5	d-Lyxose	150	C5H10O5	001114-34-7	22





Library Search Compound Report

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Sample : I4456-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

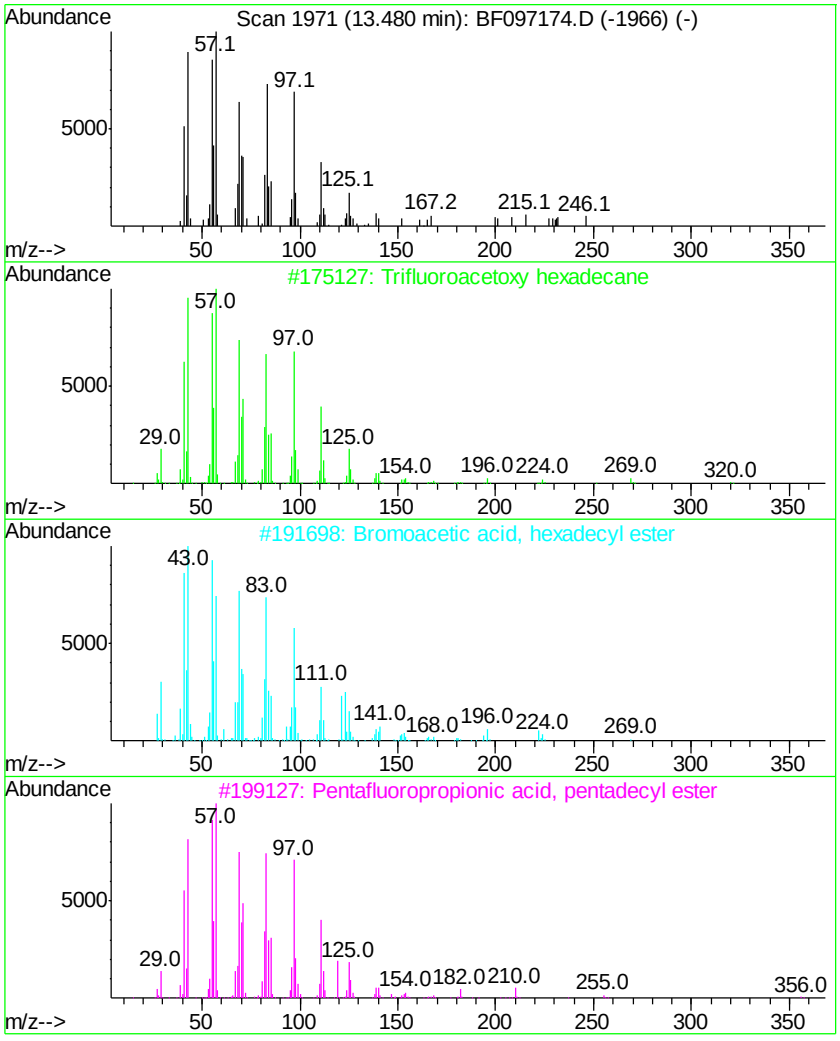
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

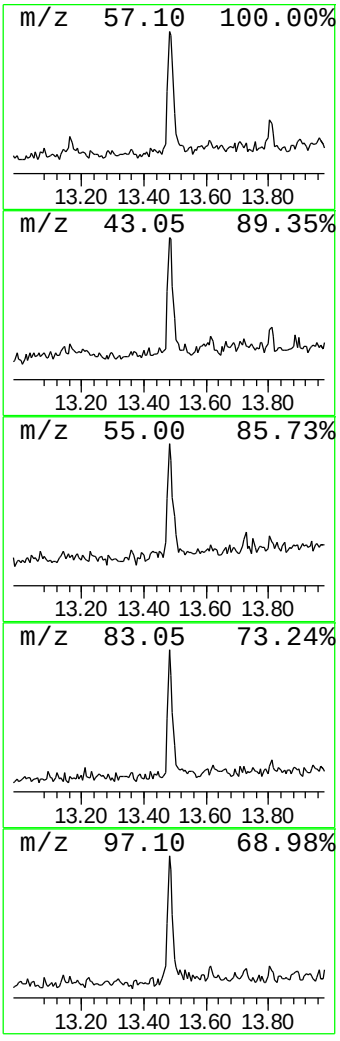
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.82 ng	132958	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
4	1-Nonadecene	266	C19H38	018435-45-5	90
5	1-Docosene	308	C22H44	001599-67-3	90





Library Search Compound Report

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Data File : BF097174.D
Acq On : 29 Jul 2017 00:42
Operator : SJ/JU
Sample : I4456-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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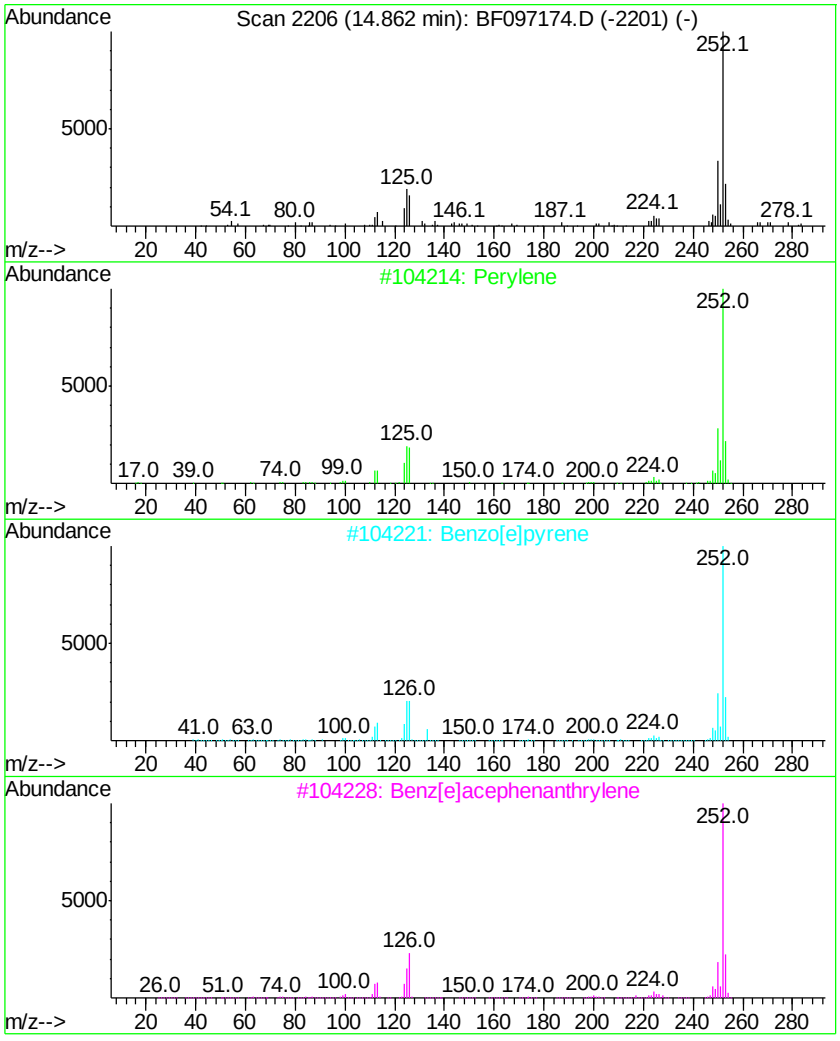
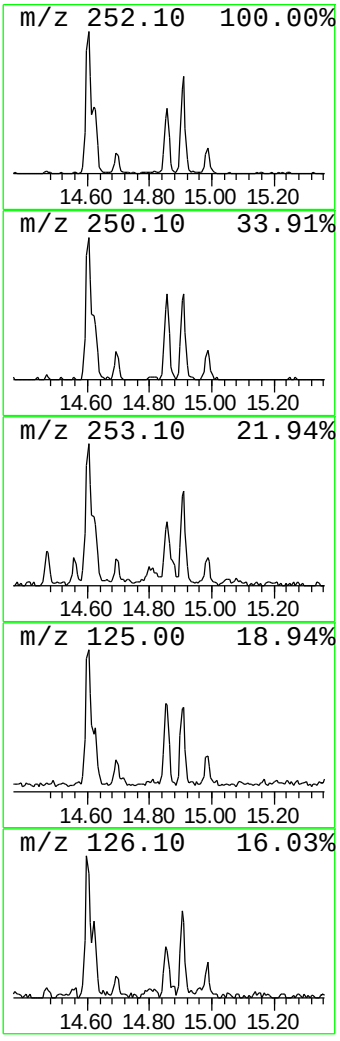
Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	5.77 ng	132704	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

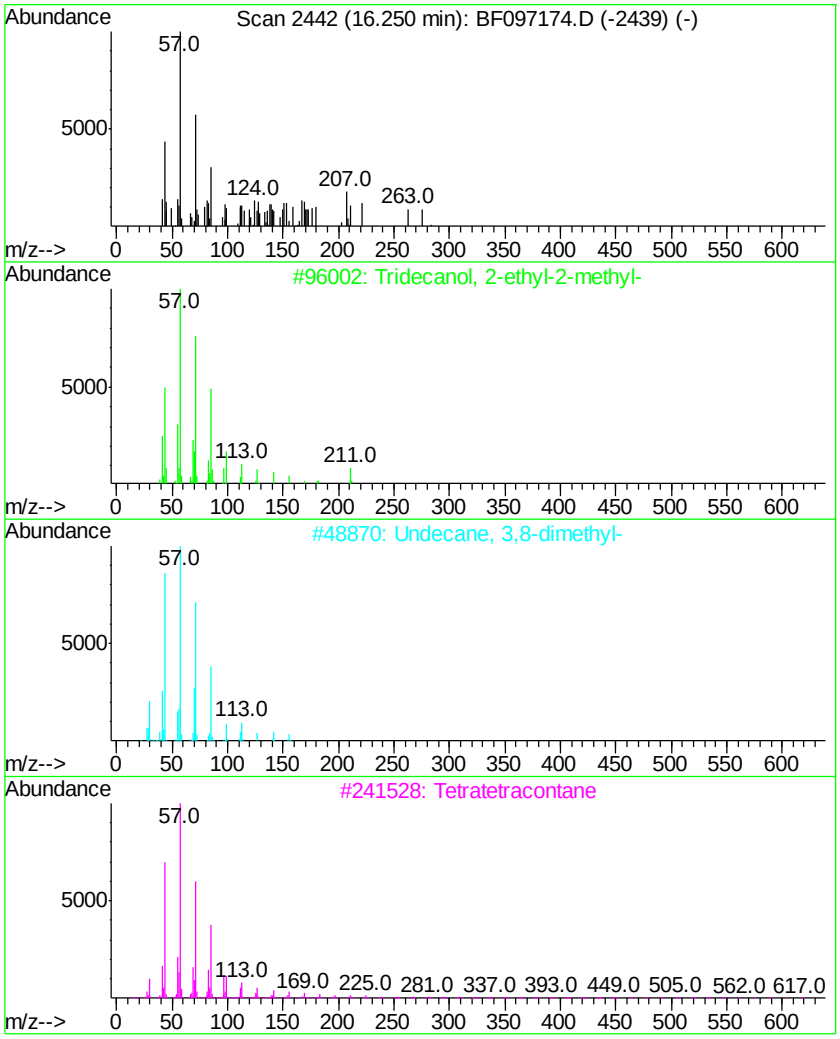
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

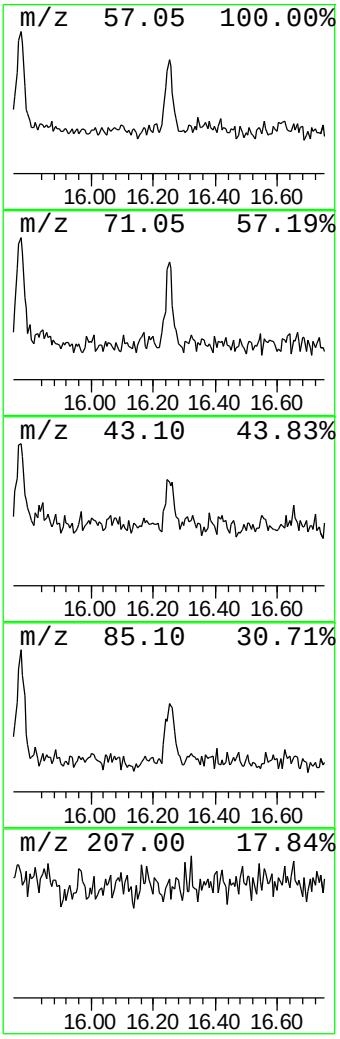
****

Peak Number 9 unknown16.25 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.00 ng	46101	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	38
2	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	35
3	Tetratetracontane	619	C44H90	007098-22-8	35
4	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	35
5	Tridecane, 5-propyl-	226	C16H34	055045-11-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097174.D
Acq On : 29 Jul 2017 00:42
Operator : SJ/JU
Sample : I4456-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-SS-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.63	22.9	ng	844579	1	6.49	738820	20.0
unknown6.26	6.26	66.5	ng	2457420	1	6.49	738820	20.0
Hexadecane	10.44	3.1	ng	84600	4	10.99	541071	20.0
Dodecanoic acid	11.54	2.9	ng	77474	4	10.99	541071	20.0
Trifluoroacetoxy ...	13.48	2.8	ng	132958	5	13.61	941684	20.0
Benzo[e]pyrene	14.86	5.8	ng	132704	6	14.96	459924	20.0
unknown16.25	16.25	2.0	ng	46101	6	14.96	459924	20.0