LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

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-BF020318.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	2.175	8	15	21	rVB	443271	620439	15.16%	1.771%
2	4.498	405	410	415	rBV	38365	45944	1.12%	0.131%
3	5.116	512	515	522	rVB	135143	164702	4.03%	0.470%
4	5.504	576	581	584	rBV	3974169	4091398	100.00%	11.677%
5	6.510	747	752	755	rBV	3576266	3902846	95.39%	11.139%
6	6.657	772	777	780	rBV	3835110	3913489	95.65%	11.170%
7	6.887	812	816	819	rBV	1160400	1021326	24.96%	2.915%
8	7.039	838	842	846	rBV	3210633	3033929	74.15%	8.659%
9	7.445	906	911	914	rBV	2674344	2623041	64.11%	7.486%
10	7.622	939	941	945	rVB	51128	45216	1.11%	0.129%
11	8.169	1030	1034	1037	rBV	1408479	1274391	31.15%	3.637%
12	9.239	1212	1216	1220	rBV	3691953	3495031	85.42%	9.975%
13	9.316	1226	1229	1231	rVB	75176	55149	1.35%	0.157%
14	9.633	1279	1283	1286	rBV	363274	324336	7.93%	0.926%
15	9.845	1311	1319	1323	rBV	214332	175595	4.29%	0.501%
16	9.922	1328	1332	1336	rBV2	1389650	1215279	29.70%	3.469%
17	10.345	1401	1404	1407	rVB	236624	173795	4.25%	0.496%
18	10.563	1437	1441	1444	rBV	51463	63362	1.55%	0.181%
19	10.710	1463	1466	1477	rVB	1798711	1830911	44.75%	5.226%
20	10.816	1481	1484	1490	rVB	156510	155786	3.81%	0.445%
21	11.269	1557	1561	1563	rBV	70737	60732	1.48%	0.173%
22	11.410	1581	1585	1588	rBV	1109475	1009431	24.67%	2.881%
23	11.433	1588	1589	1595	rVB	103461	75918	1.86%	0.217%
24	11.927	1666	1673	1678	rBV2	34757	63330	1.55%	0.181%
25	12.621	1788	1791	1795	rVB	133464	122594	3.00%	0.350%
26	12.857	1825	1831	1834	rBV	113971	129967	3.18%	0.371%
27	12.998	1850	1855	1858	rBV	2599603	2404311	58.77%	6.862%
28	13.880	2002	2005	2017	rVB	624084	602038	14.71%	1.718%
29	14.051	2029	2034	2037	rBV	1016952	986232	24.11%	2.815%
30	14.074	2037	2038	2047	rVB	78658	69314	1.69%	0.198%
31	14.515	2109	2113	2119	rBV4	47880	67285	1.64%	0.192%
32	15.098	2208	2212	2215	rBV	51485	76984	1.88%	0.220%
33	15.410	2261	2265	2271	rVB2	31522	42694	1.04%	0.122%
34	15.468	2271	2275	2281	rBV	41000	55685	1.36%	0.159%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.539	2281	2287	2295	rBV	643816	897052	21.93%	2.560%
36	15.992	2361	2364	2369	rVB3	28127	43452	1.06%	0.124%
37	16.051	2369	2374	2380	rBV2	52783	103969	2.54%	0.297%

Sum of corrected areas: 35036953

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
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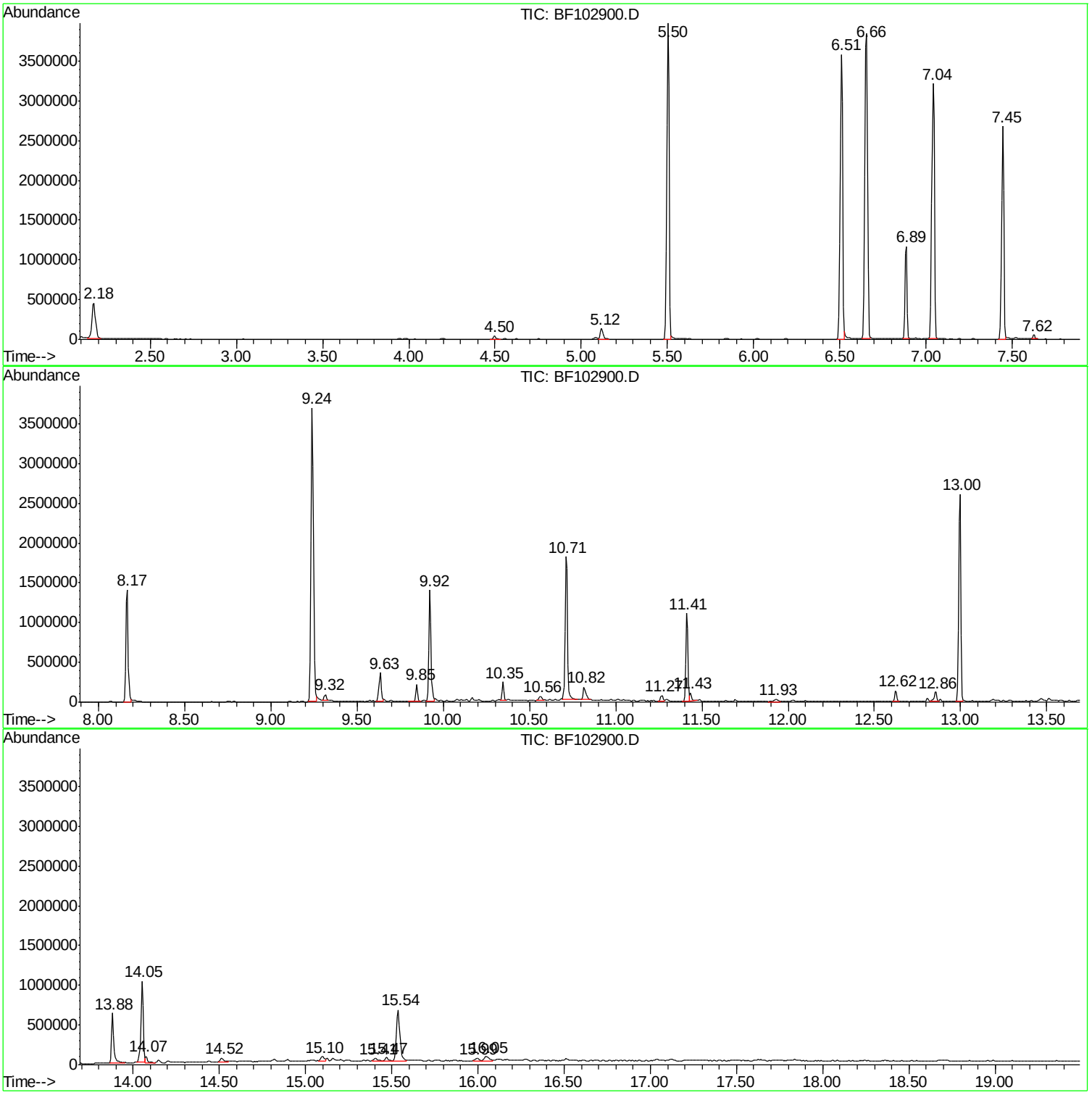
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

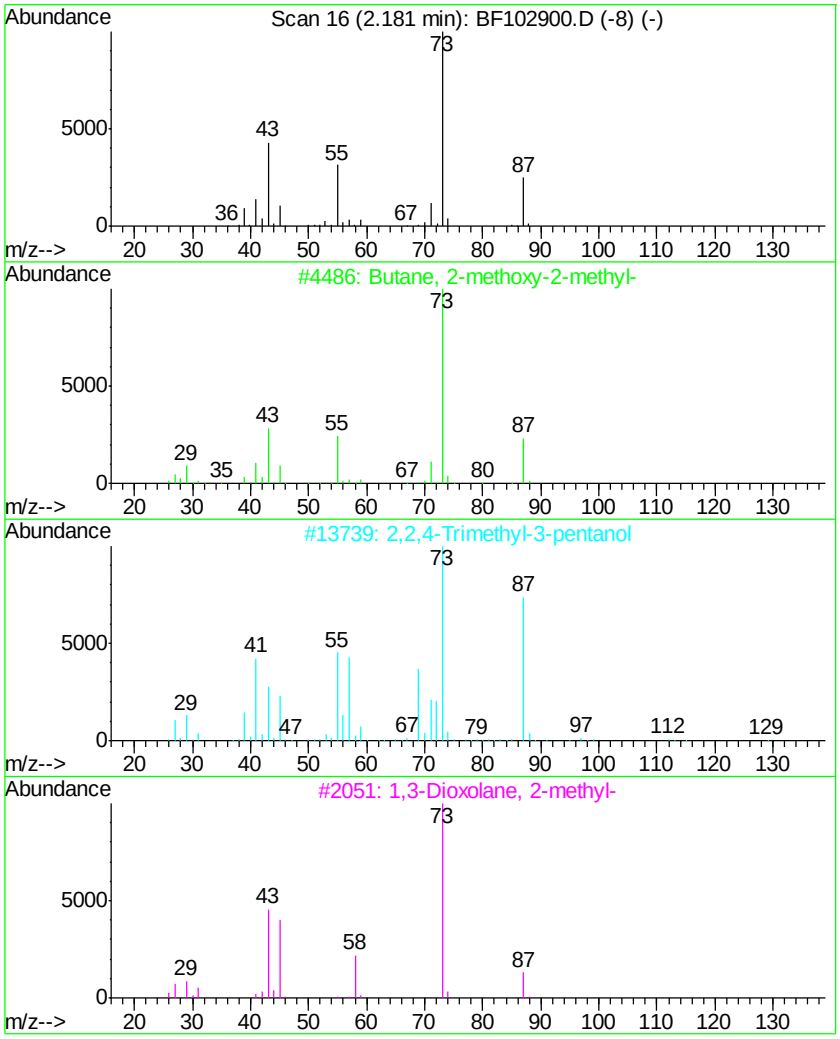
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

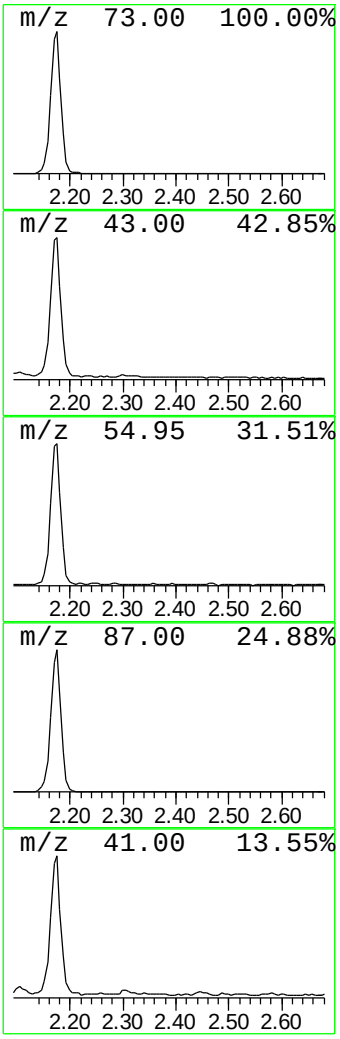
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	12.15 ng	620439	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

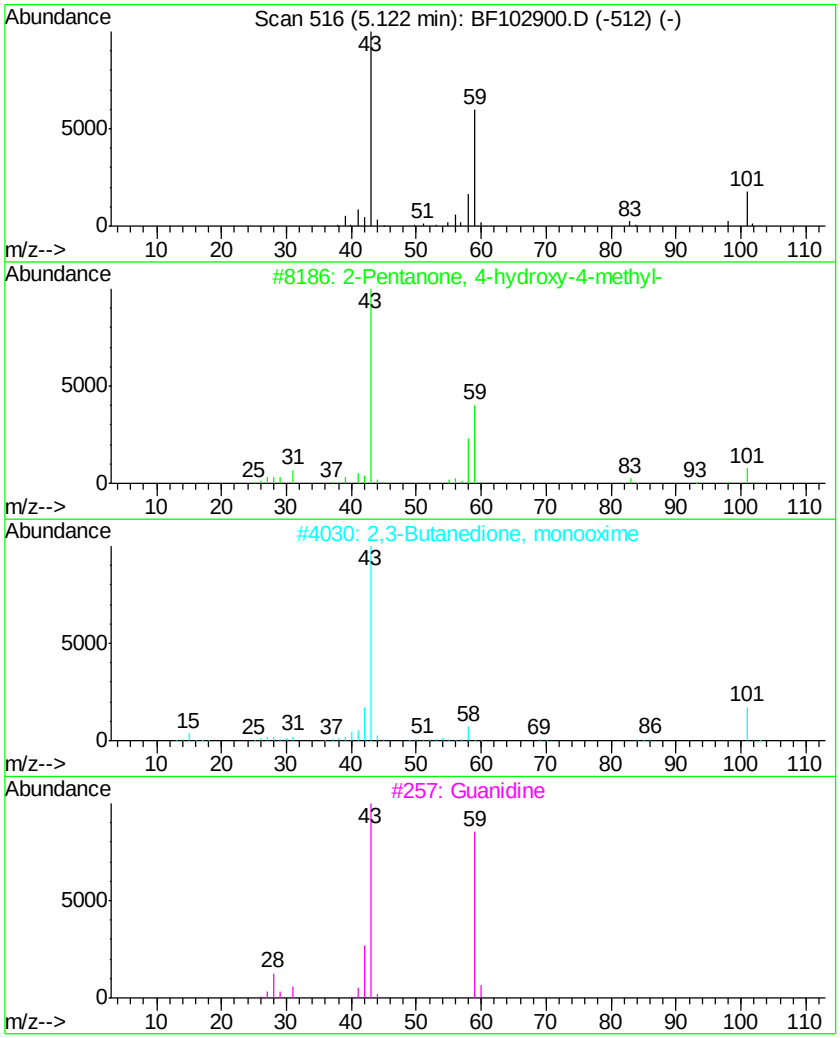
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

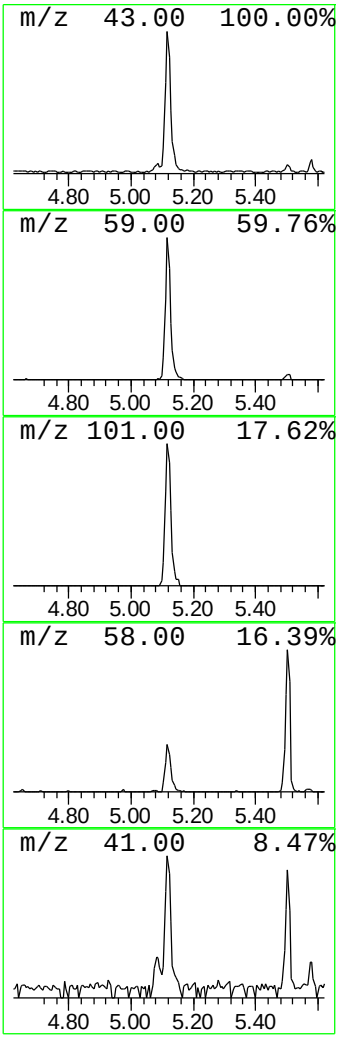
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.23 ng	164702	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Guanidine	59	CH5N3	000113-00-8	9
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

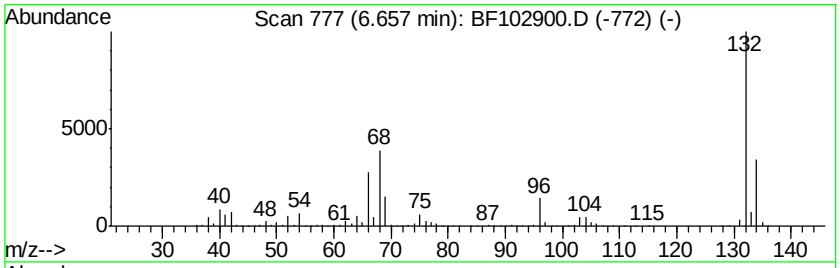
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

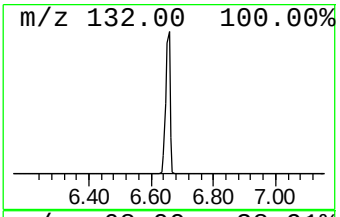
****

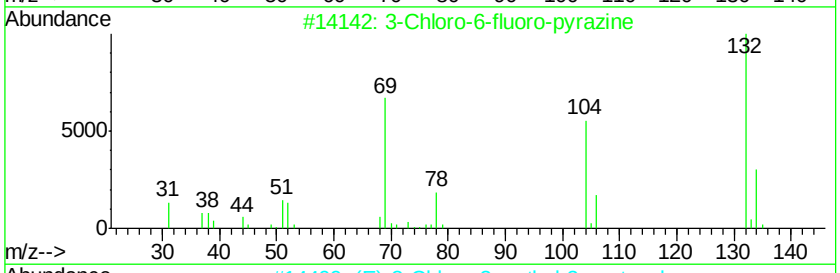
Peak Number 3 unknown6.66 Concentration Rank 1

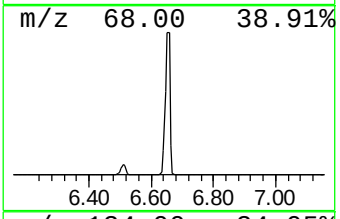
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	76.64 ng	3913490	1,4-Dichlorobenzene-d4	6.89

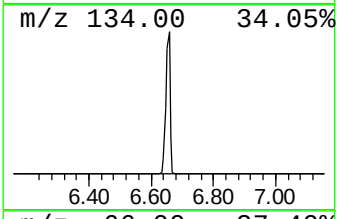
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9

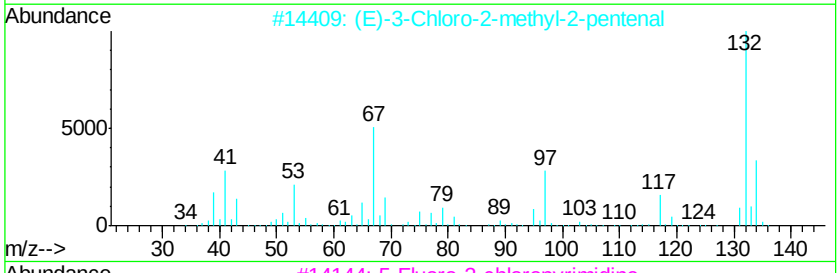


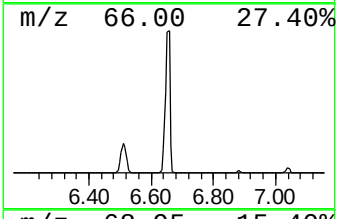


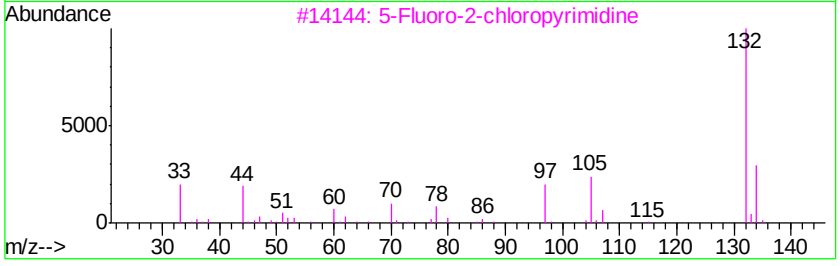


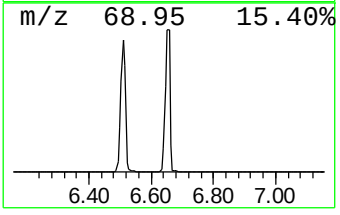












Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

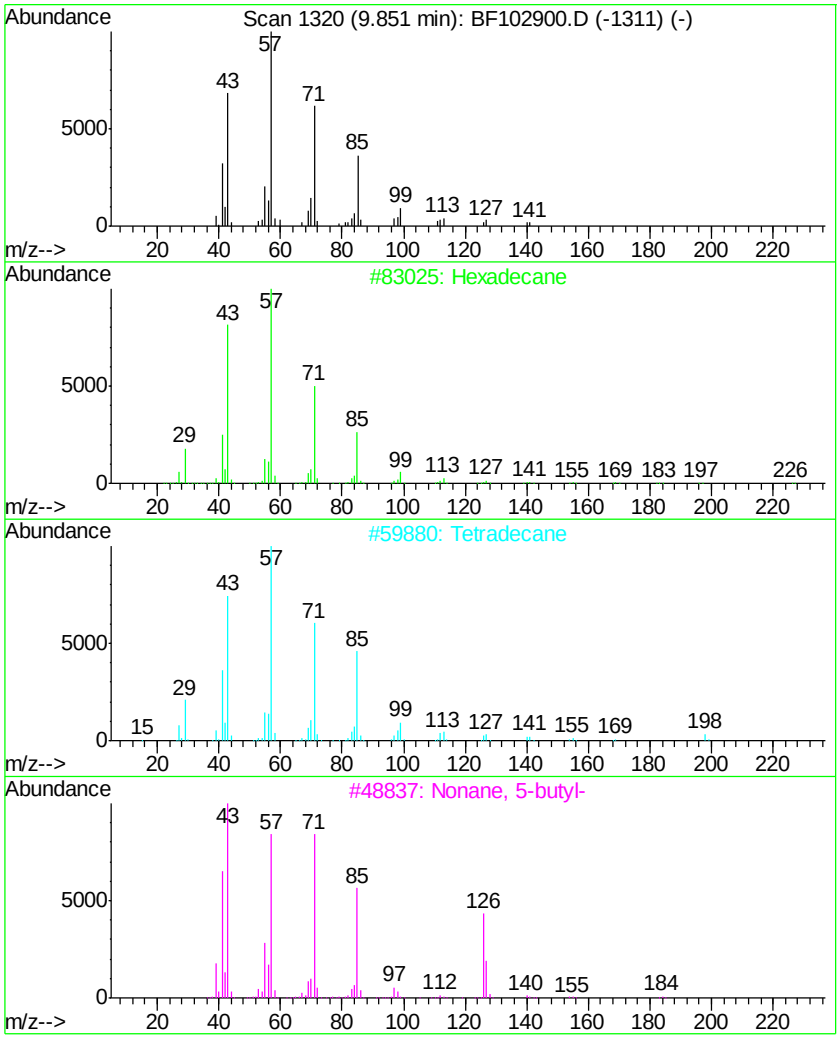
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

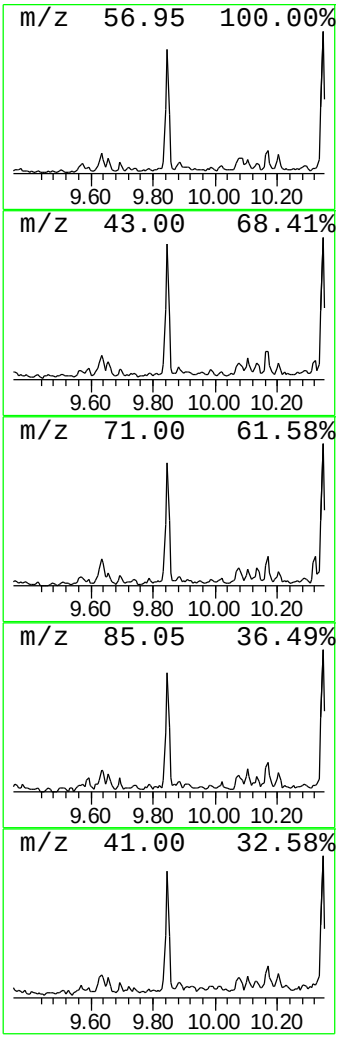
****

Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.89 ng	175595	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Nonane, 5-butyl-	184	C13H28	017312-63-9	80
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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TIC Library : C:\DATABASE\NIST11.L
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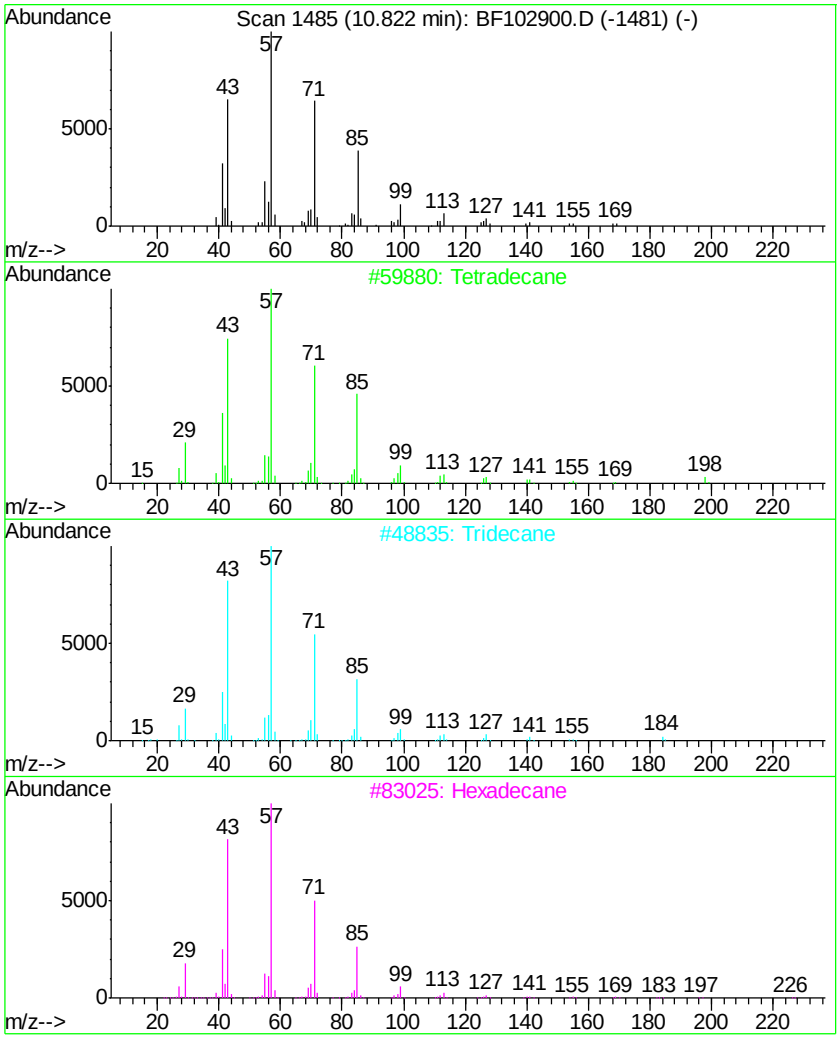
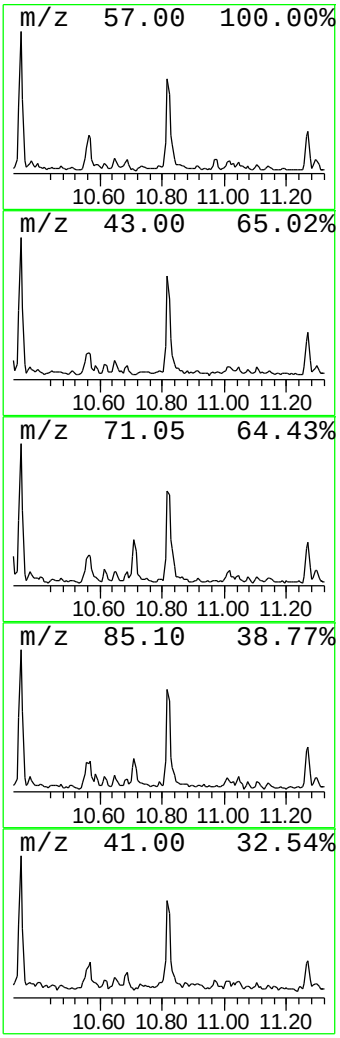
****

Peak Number 7 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.09 ng	155786	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Undecane, 6-ethyl-	184	C13H28	017312-60-6	78
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78





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Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

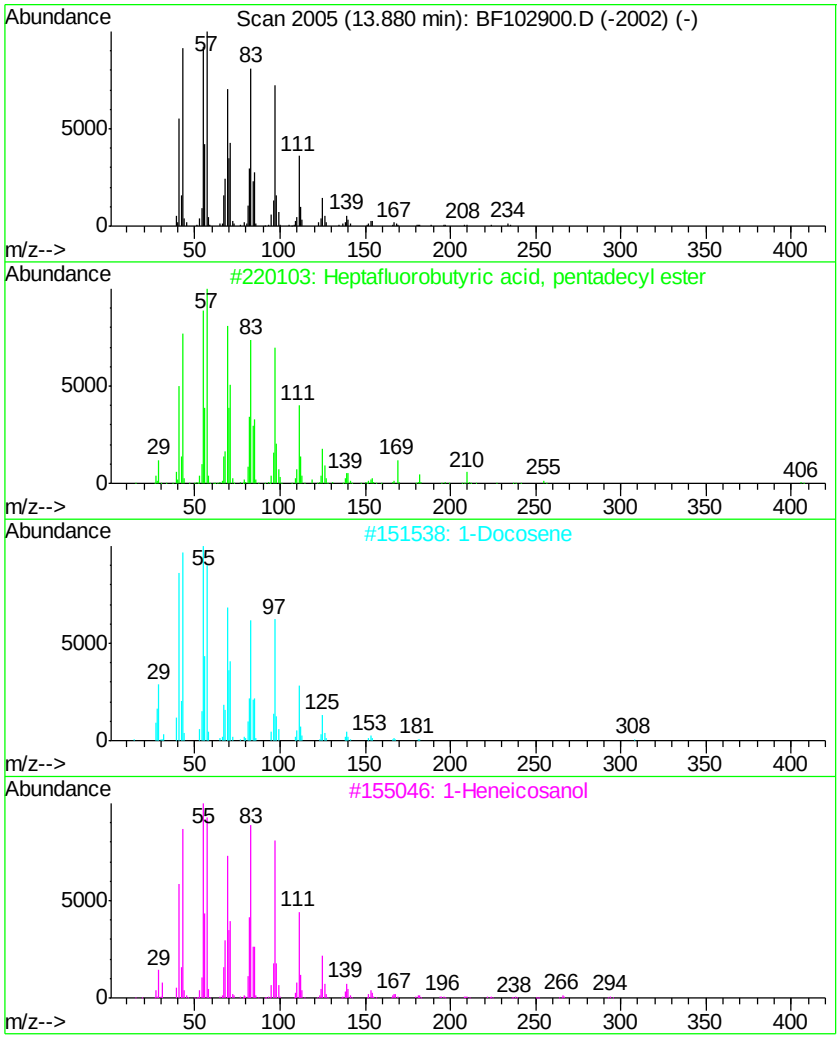
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

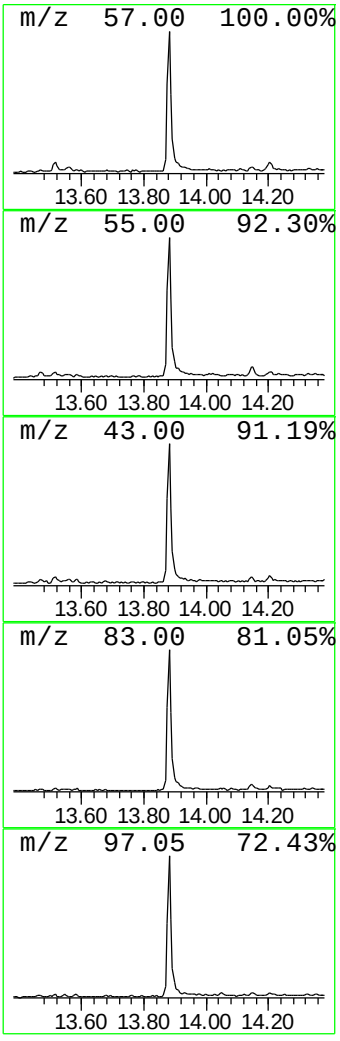
****

Peak Number 8 Heptafluorobutyric acid, pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	12.21 ng	602038	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5	1-Nonadecene	266	C19H38	018435-45-5	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
Sample : J1506-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-20(8-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

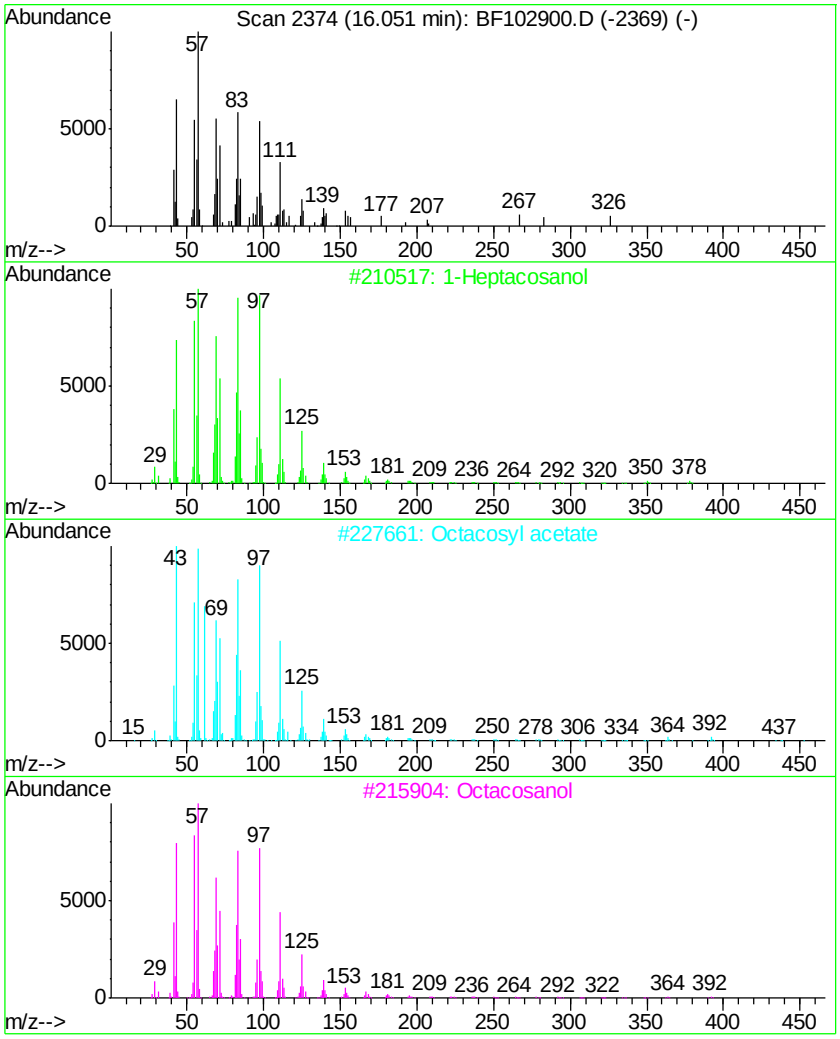
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

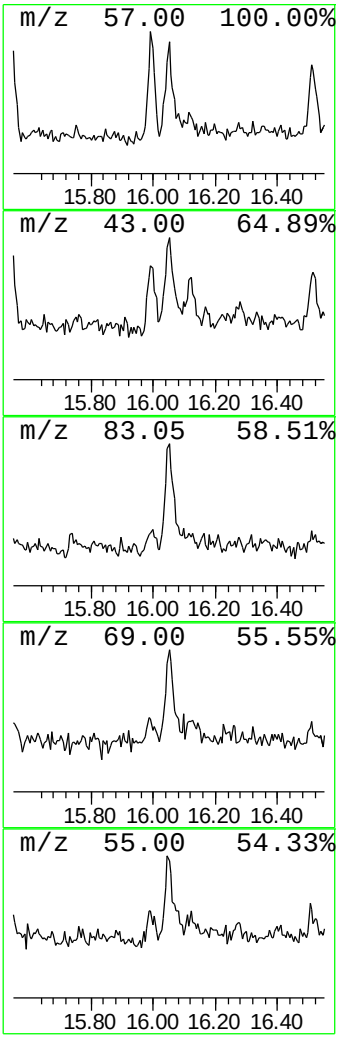
****

Peak Number 9 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	2.32 ng	103969	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Octacosyl acetate	452	C30H60O2	018206-97-8	94
3	Octacosanol	410	C28H58O	000557-61-9	93
4	Triacontyl acetate	480	C32H64O2	041755-58-2	91
5	2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102900.D
Acq On : 9 Feb 2018 20:26
Operator : SJ/JU
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.18	12.2	ng	620439	1	6.89	1021330	20.0
2-Pentanone, 4-hy...	5.12	3.2	ng	164702	1	6.89	1021330	20.0
unknown6.66	6.66	76.6	ng	3913490	1	6.89	1021330	20.0
Hexadecane	9.85	2.9	ng	175595	3	9.92	1215280	20.0
Tetradecane	10.82	3.1	ng	155786	4	11.41	1009430	20.0
Heptafluorobutyri...	13.88	12.2	ng	602038	5	14.05	986232	20.0
1-Heptacosanol	16.05	2.3	ng	103969	6	15.54	897052	20.0