LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127186.D
Acq On : 03 Mar 2022 22:20
Operator : CG\JU
Sample : N1726-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 275

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127186.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.528	193	211	226	rBV	244139	941626	33.82%	4.510%
2	5.128	479	483	491	rVB	24850	32643	1.17%	0.156%
3	5.522	545	550	553	rBV	2988971	2760116	99.14%	13.221%
4	6.528	716	721	724	rBV	2770529	2784151	100.00%	13.336%
5	6.887	779	782	786	rBV	684169	604154	21.70%	2.894%
6	7.457	874	879	882	rBV	1817487	1625184	58.37%	7.785%
7	8.069	980	983	993	rBV	205394	212236	7.62%	1.017%
8	8.175	997	1001	1004	rBV	968203	782266	28.10%	3.747%
9	8.322	1022	1026	1035	rBV	30852	74820	2.69%	0.358%
10	9.251	1178	1184	1187	rBV	3231381	2649888	95.18%	12.693%
11	9.739	1262	1267	1274	rBV2	29055	51867	1.86%	0.248%
12	9.934	1296	1300	1303	rBV	958612	768272	27.59%	3.680%
13	10.328	1362	1367	1368	rBV	41203	37713	1.35%	0.181%
14	10.345	1368	1370	1374	rVB	41716	36211	1.30%	0.173%
15	10.722	1430	1434	1438	rBV	1848664	1641995	58.98%	7.865%
16	10.928	1465	1469	1474	rBV4	24459	32666	1.17%	0.156%
17	11.363	1540	1543	1547	rVB	74016	59255	2.13%	0.284%
18	11.422	1549	1553	1556	rVV	816043	692827	24.88%	3.319%
19	11.445	1556	1557	1562	rVB	85253	57707	2.07%	0.276%
20	11.580	1577	1580	1586	rBV2	40697	45580	1.64%	0.218%
21	11.804	1614	1618	1621	rVB	114315	104331	3.75%	0.500%
22	11.927	1636	1639	1642	rBV4	25724	33219	1.19%	0.159%
23	12.039	1655	1658	1663	rVB3	23291	35352	1.27%	0.169%
24	12.463	1726	1730	1737	rBV	774982	1325919	47.62%	6.351%
25	12.598	1750	1753	1757	rBV5	27616	33473	1.20%	0.160%
26	12.639	1757	1760	1765	rVV	101686	102838	3.69%	0.493%
27	12.786	1782	1785	1788	rVB3	49242	49682	1.78%	0.238%
28	12.869	1793	1799	1802	rBV	110508	118920	4.27%	0.570%
29	13.010	1819	1823	1826	rVB	2216089	1780802	63.96%	8.530%
30	13.069	1831	1833	1840	rVB7	30789	39981	1.44%	0.192%
31	13.192	1849	1854	1857	rBV3	22555	36598	1.31%	0.175%
32	13.916	1972	1977	1980	rBV4	63416	98195	3.53%	0.470%
33	14.069	1998	2003	2005	rBV	529944	493024	17.71%	2.362%
34	14.092	2005	2007	2010	rVB	96904	78899	2.83%	0.378%
35	15.121	2179	2182	2185	rBV2	51355	57343	2.06%	0.275%
36	15.563	2253	2257	2271	rVB2	399449	531292	19.08%	2.545%

LSC Area Percent Report

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Operator : CG\JU
Sample : N1726-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
275

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.010	2330	2333	2338	rVB	44988	65854	2.37%	0.315%

Sum of corrected areas: 20876899

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Data File : BF127186.D
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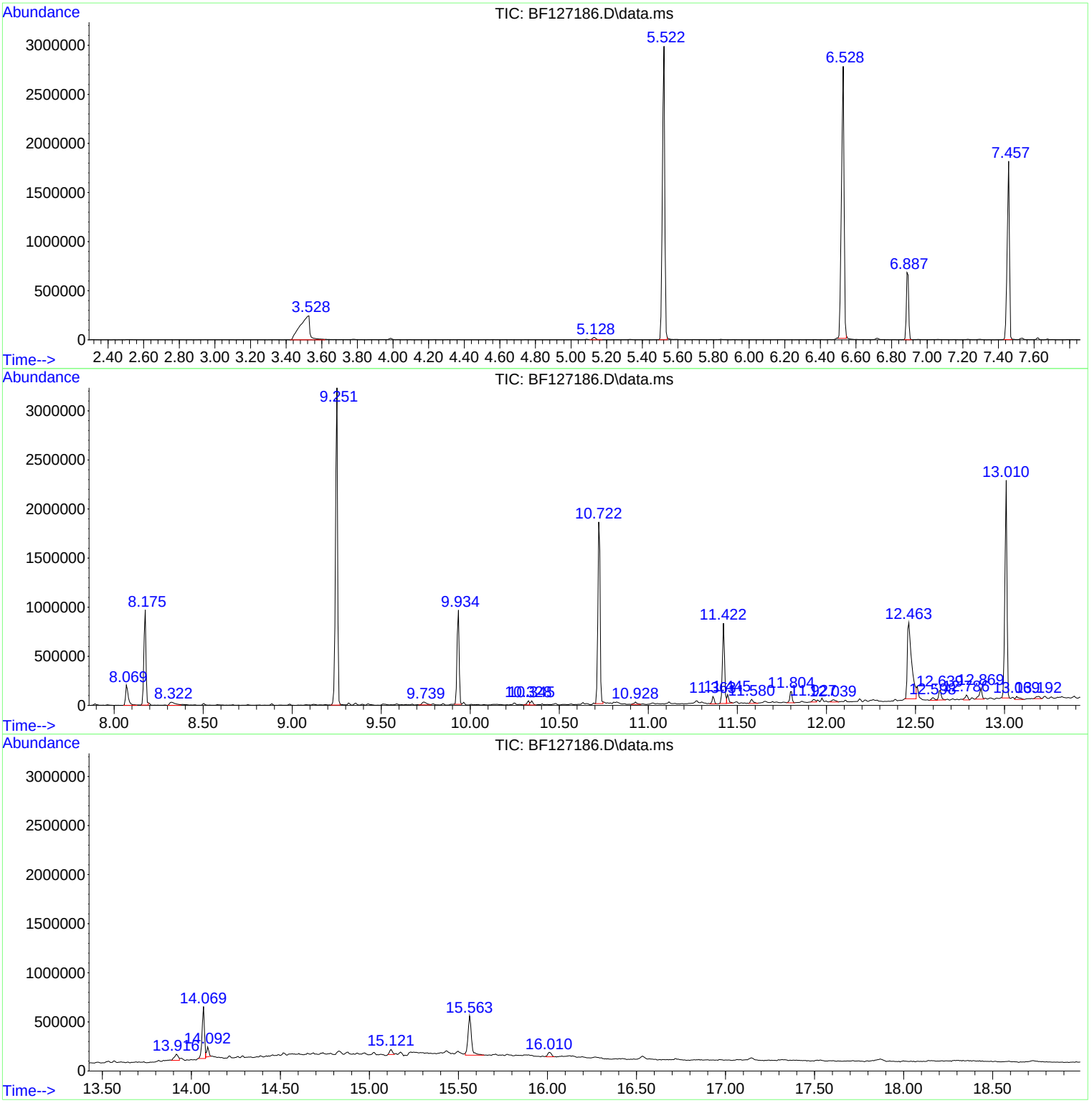
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127186.D
Acq On : 03 Mar 2022 22:20
Operator : CG\JU
Sample : N1726-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

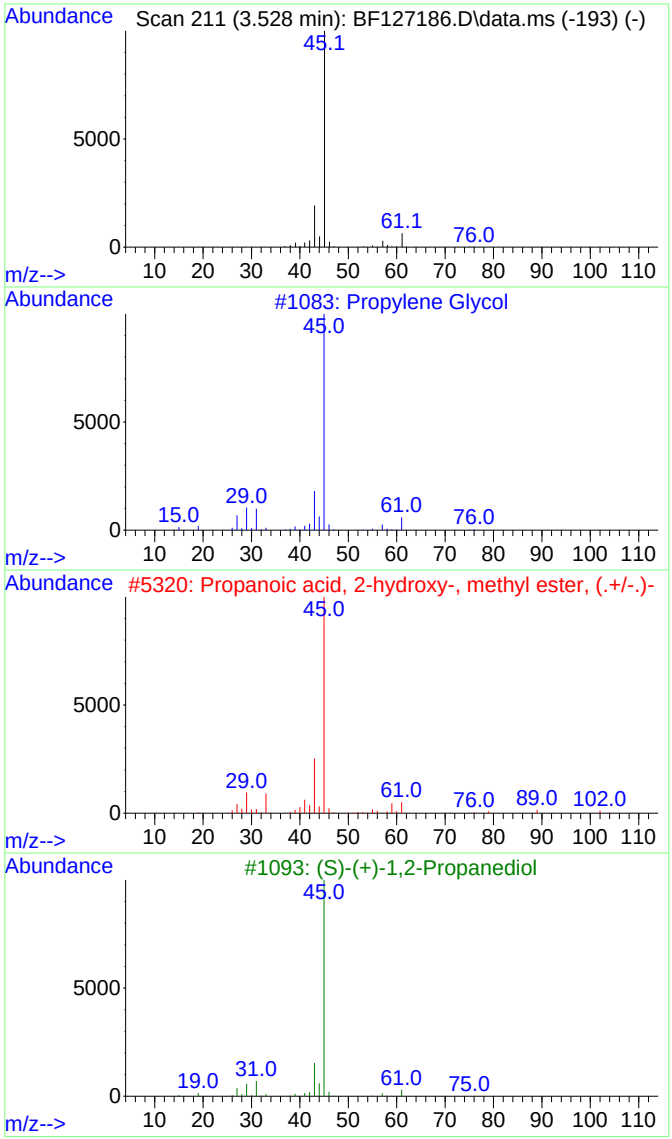
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

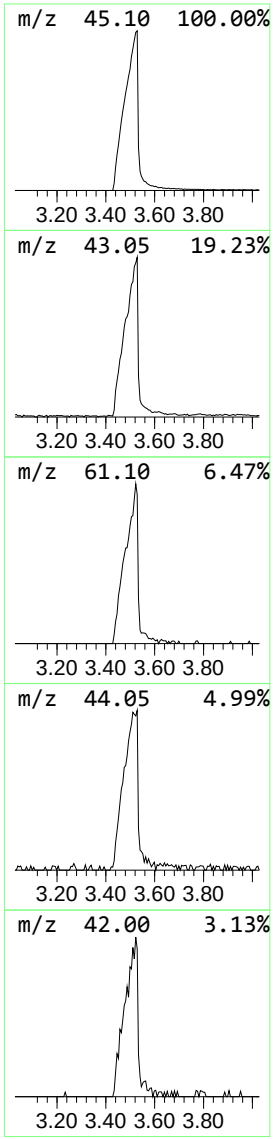
****

Peak Number 1 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.528	31.17 ng	941626	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





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Operator : CG\JU
Sample : N1726-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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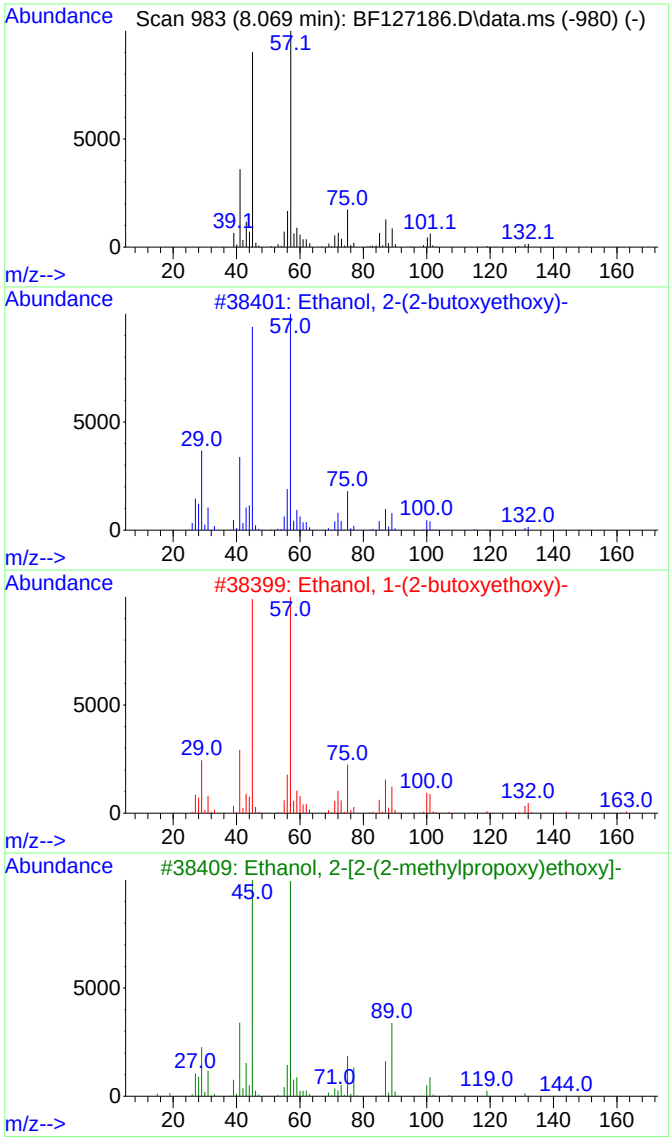
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

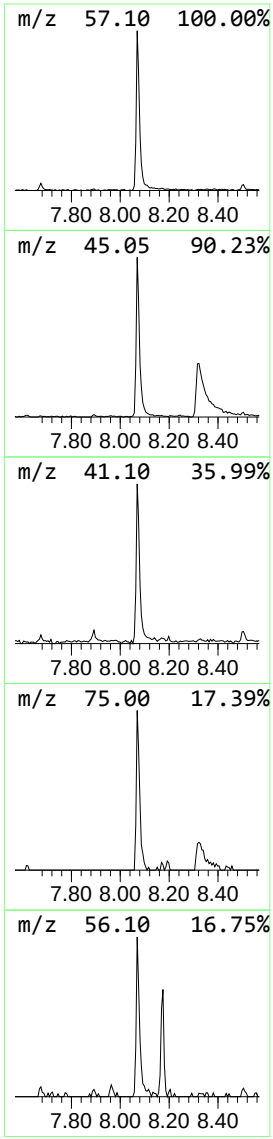
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	5.43 ng	212236	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	86
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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Instrument :
BNA_F
ClientSampleId :
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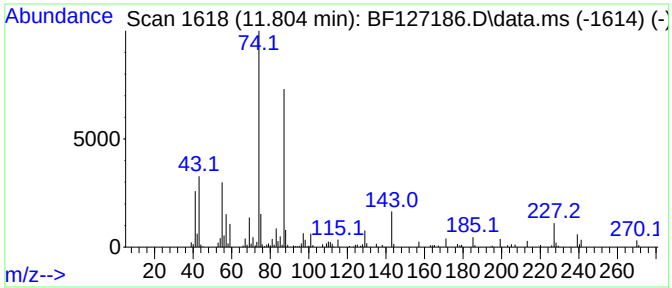
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

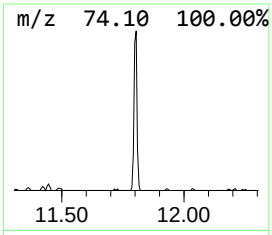
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

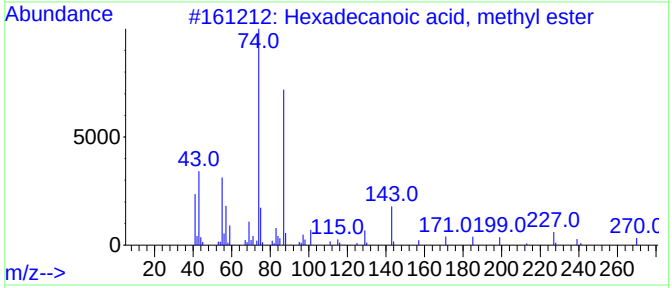
****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

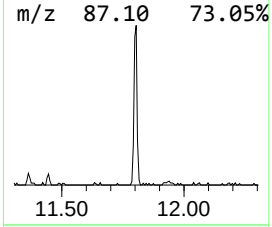
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	3.01 ng	104331	Phenanthrene-d10	11.422

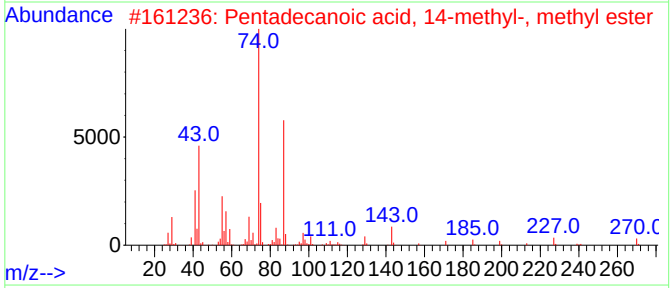
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	76

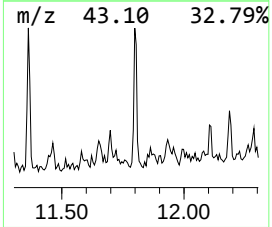


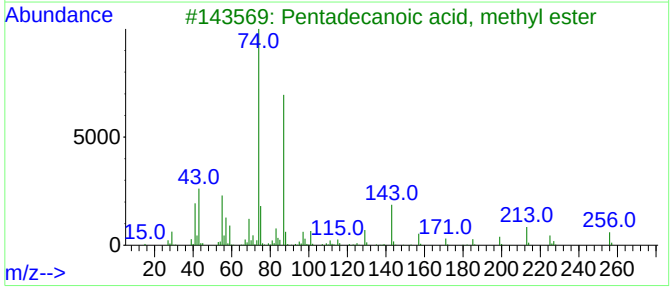


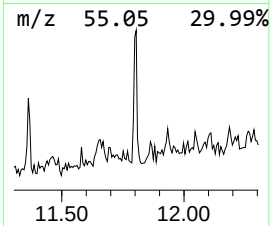


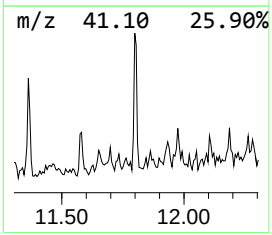












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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

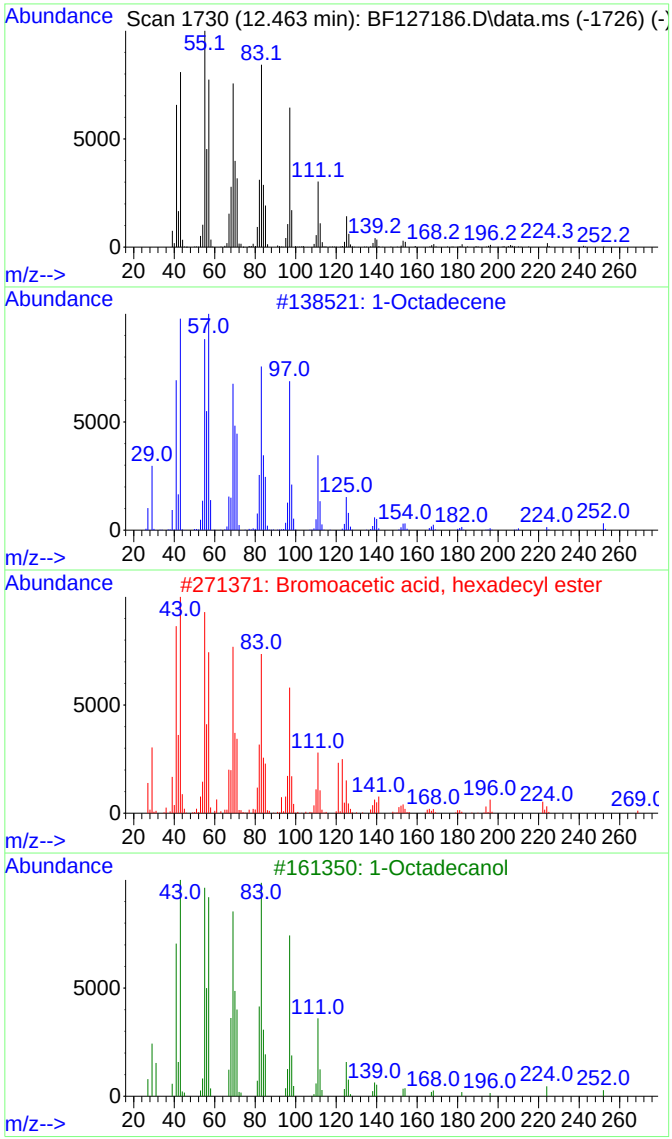
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

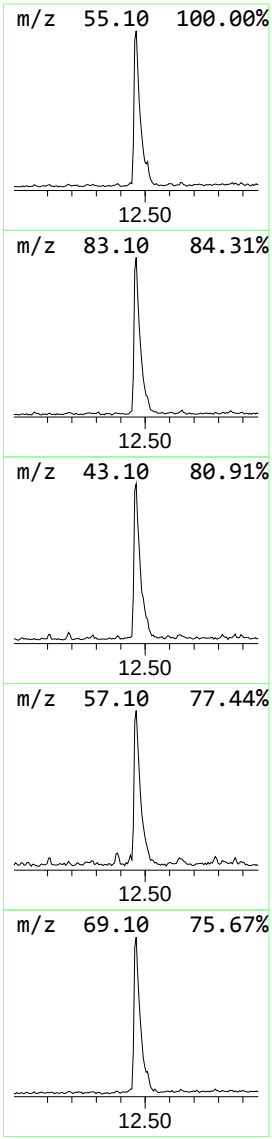
****

Peak Number 4 1-Octadecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	38.28 ng	1325920	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	96
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	1-Octadecanol	270	C18H38O	000112-92-5	94
4	1-Hexadecanol	242	C16H34O	036653-82-4	94
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	94





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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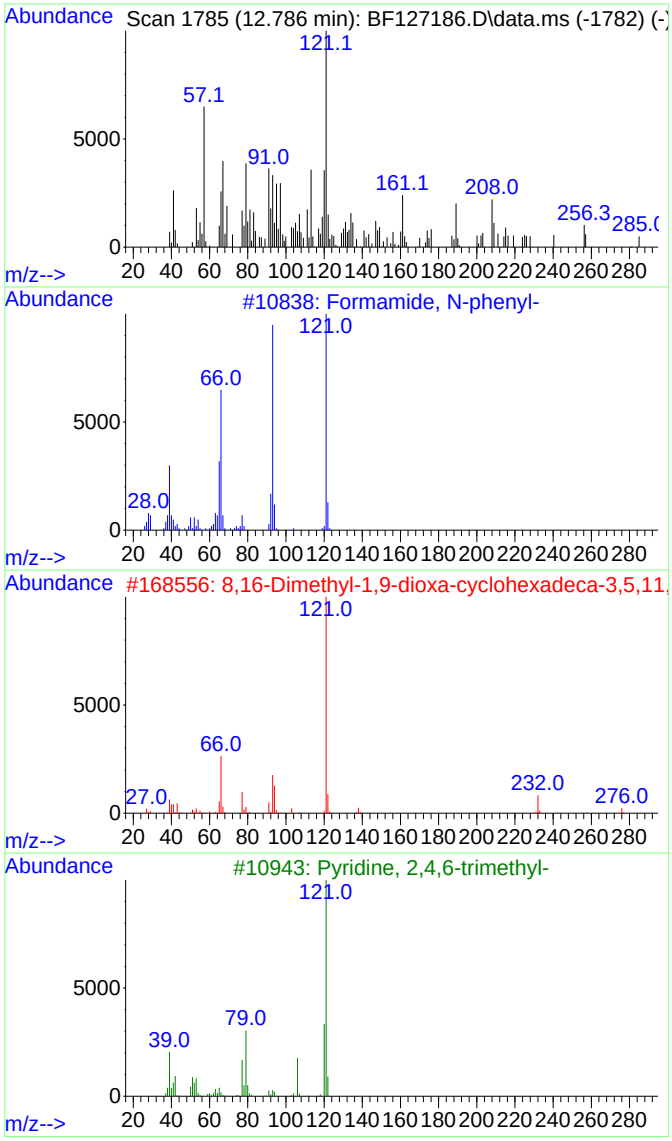
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

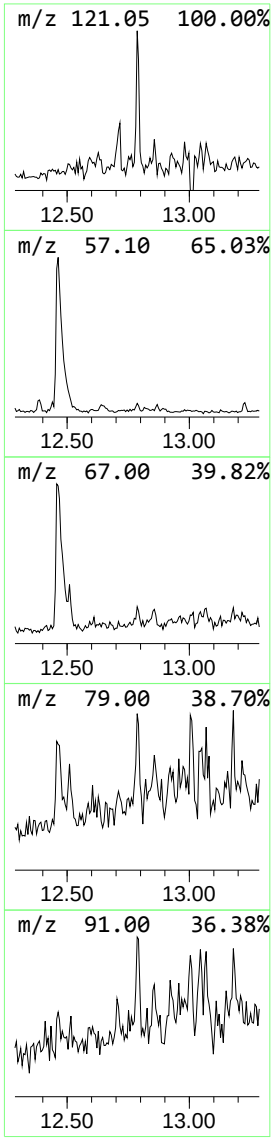
****

Peak Number 5 unknown12.786 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	2.02 ng	49682	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formamide, N-phenyl-	121	C7H7NO	000103-70-8	38
2	8,16-Dimethyl-1,9-dioxa-cyclohex...	276	C16H20O4	1000185-93-1	35
3	Pyridine, 2,4,6-trimethyl-	121	C8H11N	000108-75-8	27
4	cis-anti-trans-Tricyclo[7.3.0.0(...	164	C12H20	030159-13-8	27
5	cis-syn-cis-Tricyclo[7.3.0.0(2,6...	164	C12H20	030159-14-9	27





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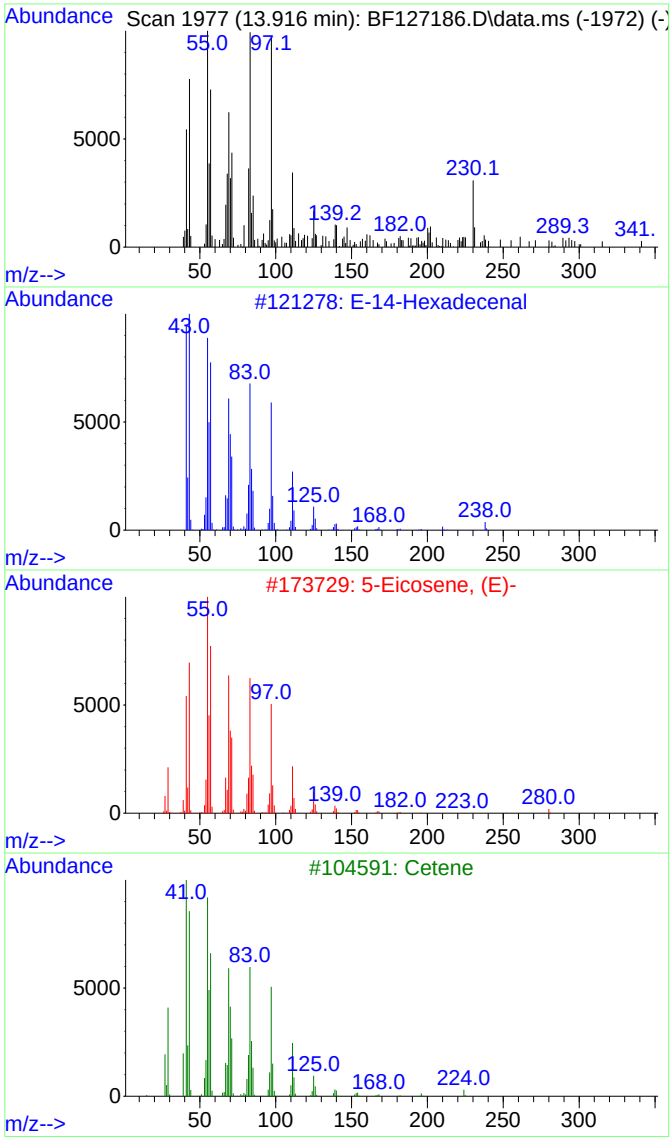
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

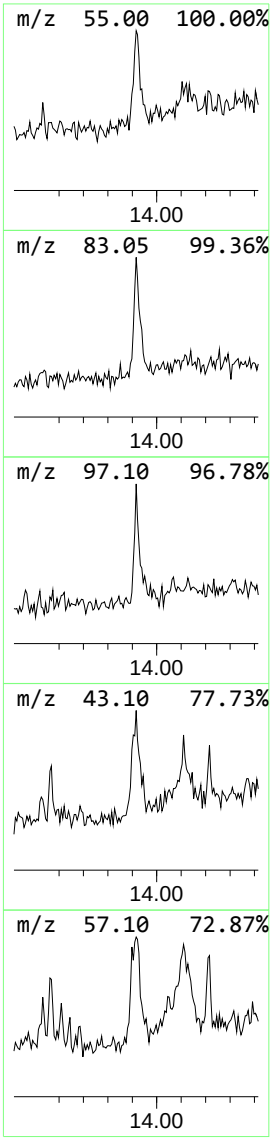
****

Peak Number 6 E-14-Hexadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	3.98 ng	98195	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	83
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	78
3	Cetene	224	C16H32	000629-73-2	64
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	60
5	1-Heptadecene	238	C17H34	006765-39-5	60





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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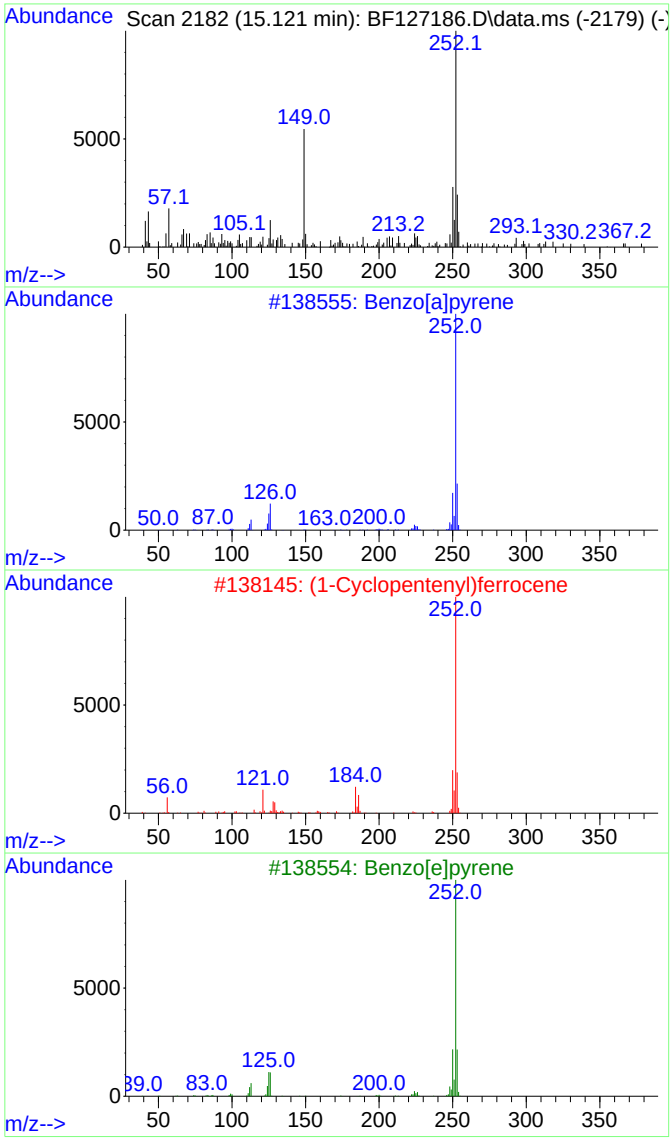
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

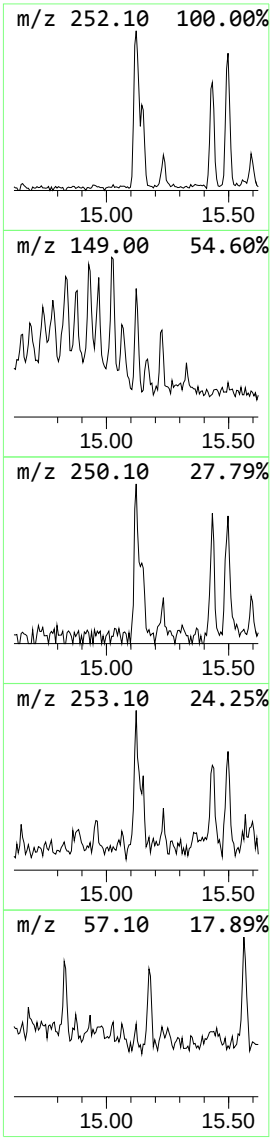
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (1-Cyclopentenyl)ferrocene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	2.16 ng	57343	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	53
2	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	53
3	Benzo[e]pyrene	252	C20H12	000192-97-2	49
4	Benzo[b]naphtho[2,3-d]thiophene,...	252	C17H16S	024964-06-5	47
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	47





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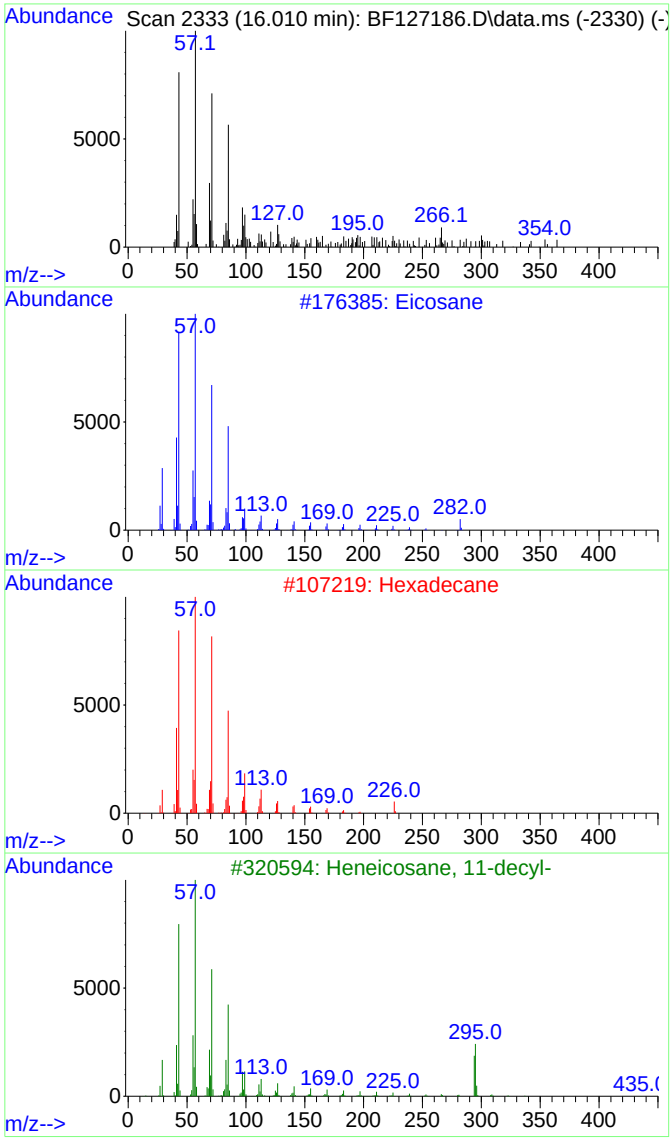
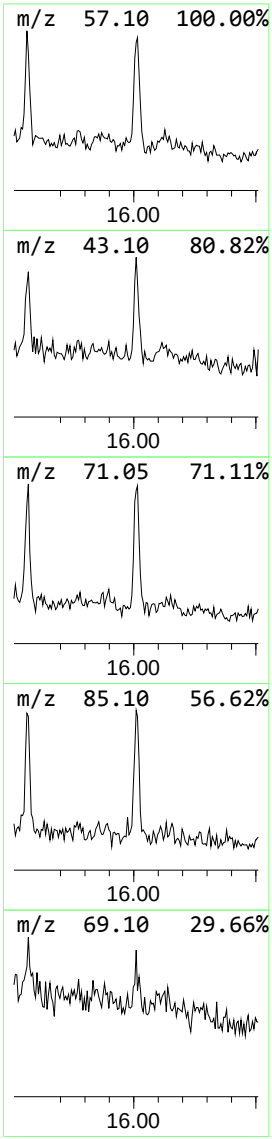
****

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	2.48 ng	65854	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	Hexadecane	226	C16H34	000544-76-3	53
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	53
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	53
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127186.D
Acq On : 03 Mar 2022 22:20
Operator : CG\JU
Sample : N1726-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
275

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propylene Glycol	3.528	31.2	ng	941626	1	6.893	604154	20.0
Ethanol, 2-(2-b...	8.069	5.4	ng	212236	2	8.175	782266	20.0
Hexadecanoic ac...	11.804	3.0	ng	104331	4	11.422	692827	20.0
1-Octadecene	12.463	38.3	ng	1325920	4	11.422	692827	20.0
unknown12.786	12.786	2.0	ng	49682	5	14.069	493024	20.0
E-14-Hexadecenal	13.916	4.0	ng	98195	5	14.069	493024	20.0
(1-Cyclopenteny...	15.121	2.2	ng	57343	6	15.563	531292	20.0
Eicosane	16.010	2.5	ng	65854	6	15.563	531292	20.0