LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095041.D
Acq On : 10 May 2017 1:28
Operator : SJ/MA
Sample : I3027-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4-5-6-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-BF050217.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	4.107	365	369	382	rBV	33481	81933	3.32%	0.388%
2	5.031	522	526	547	rBV	203194	397797	16.12%	1.882%
3	5.666	629	634	658	rBV	1288654	2123004	86.03%	10.046%
4	7.260	900	905	920	rBV	1381112	2074370	84.06%	9.815%
5	7.378	920	925	943	rVB	1689018	2401942	97.33%	11.365%
6	7.713	978	982	993	rBV	478193	564633	22.88%	2.672%
7	7.948	1017	1022	1038	rBV	1514144	1739674	70.50%	8.232%
8	8.613	1130	1135	1159	rBV	947468	1327625	53.80%	6.282%
9	9.730	1321	1325	1342	rBV	572833	757502	30.70%	3.584%
10	11.507	1621	1627	1642	rBV	1962537	2467747	100.00%	11.677%
11	12.201	1741	1745	1755	rBV	128309	169026	6.85%	0.800%
12	12.560	1801	1806	1818	rBV2	565723	839181	34.01%	3.971%
13	13.401	1945	1949	1955	rVB	32579	34228	1.39%	0.162%
14	13.860	2021	2027	2042	rBV	884261	1341223	54.35%	6.346%
15	14.171	2077	2080	2083	rBV	41747	49731	2.02%	0.235%
16	14.906	2201	2205	2210	rBV	21613	25332	1.03%	0.120%
17	14.959	2210	2214	2228	rVB	539497	750064	30.39%	3.549%
18	15.930	2373	2379	2391	rBV2	115425	155863	6.32%	0.738%
19	17.018	2560	2564	2576	rBV3	40145	60650	2.46%	0.287%
20	17.289	2605	2610	2619	rBV	1600649	1844993	74.76%	8.730%
21	17.983	2720	2728	2739	rBV	511652	623110	25.25%	2.948%
22	18.089	2743	2746	2753	rVB2	22576	32336	1.31%	0.153%
23	18.530	2817	2821	2834	rBV3	54470	119194	4.83%	0.564%
24	18.630	2834	2838	2847	rVV	488190	553894	22.45%	2.621%
25	19.653	3009	3012	3015	rBV3	22277	28294	1.15%	0.134%
26	20.294	3117	3121	3130	rVB	395106	570394	23.11%	2.699%

Sum of corrected areas: 21133740

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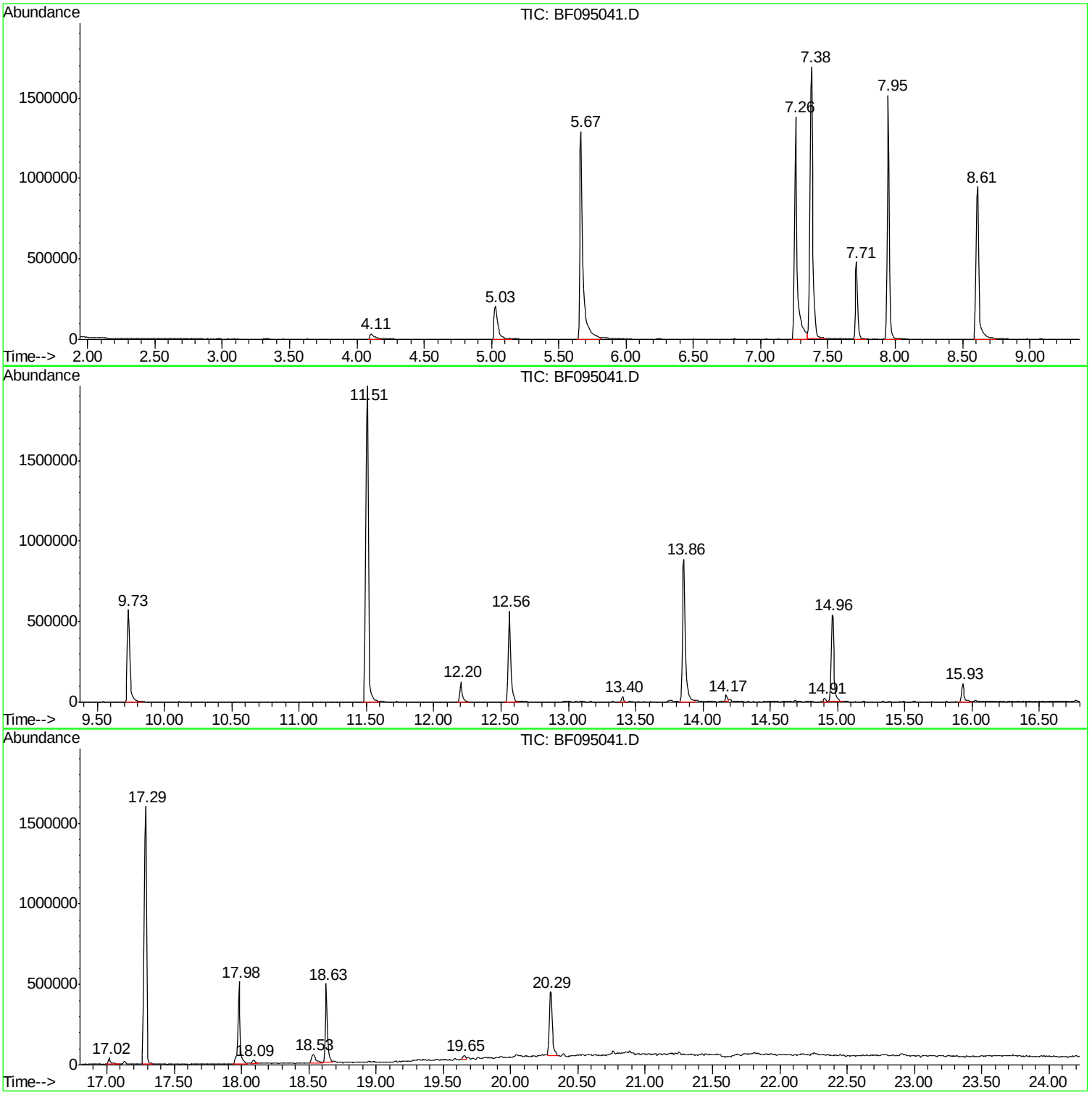
Instrument : BNA_F
ClientSampleId : TP-4-5-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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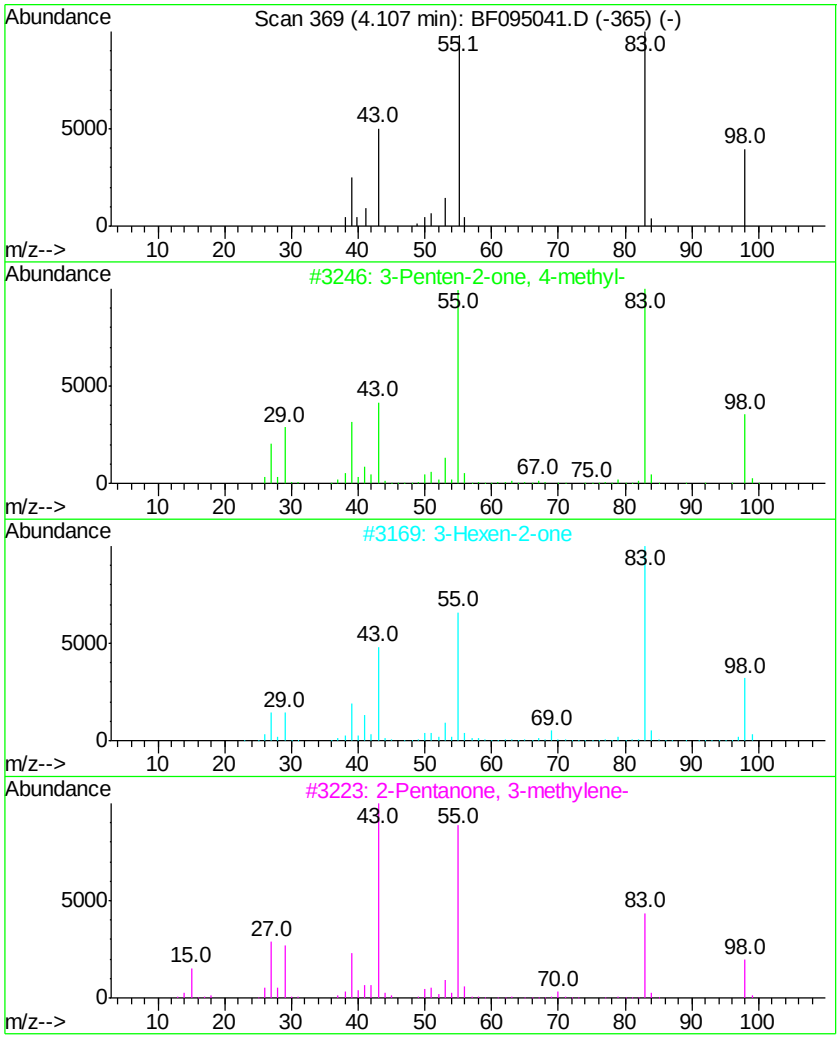
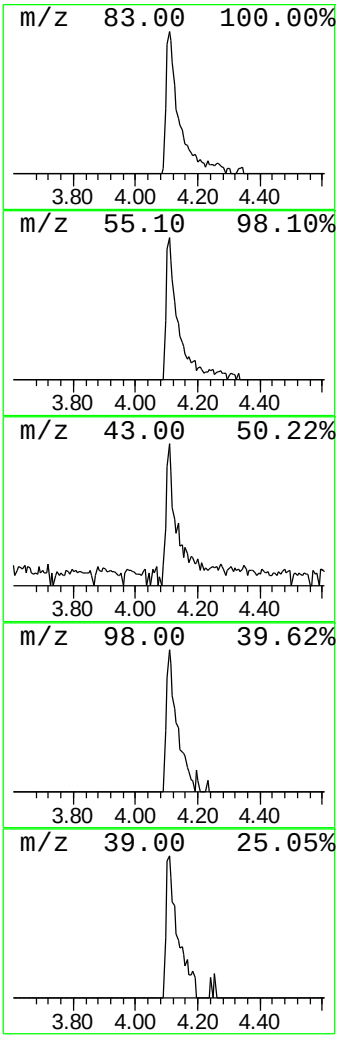
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	2.90 ng	81933	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	83
3	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	83
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





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Sample : I3027-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4-5-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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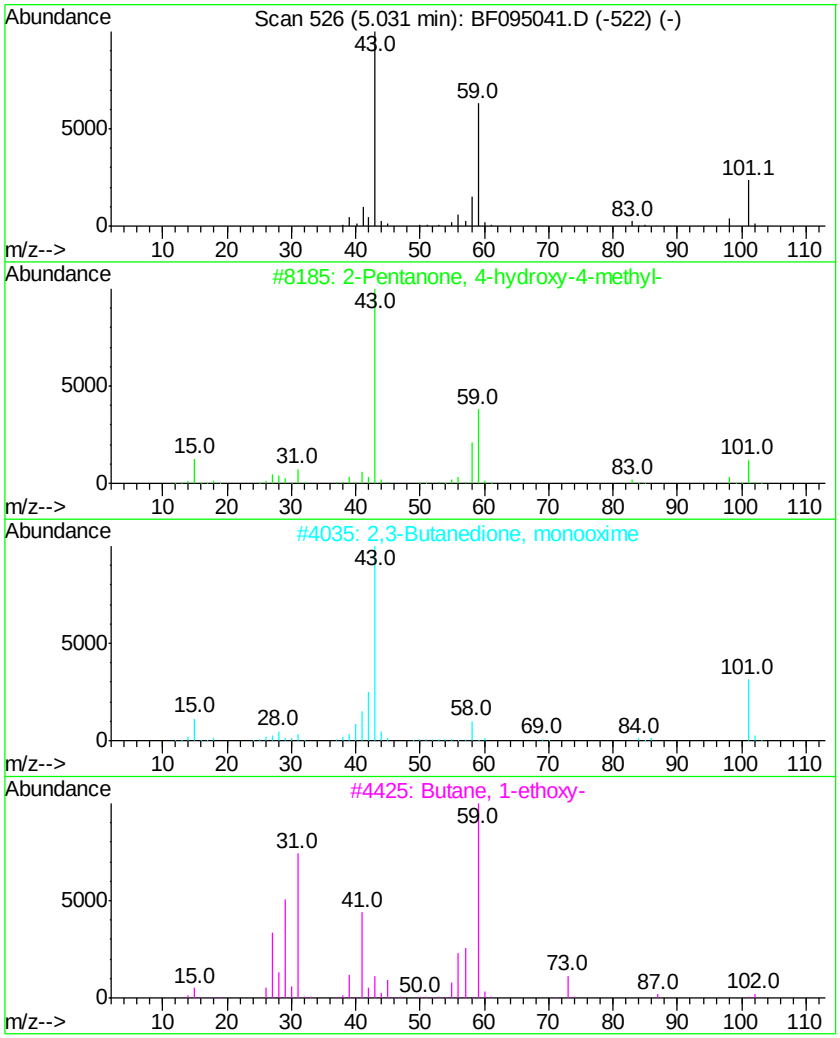
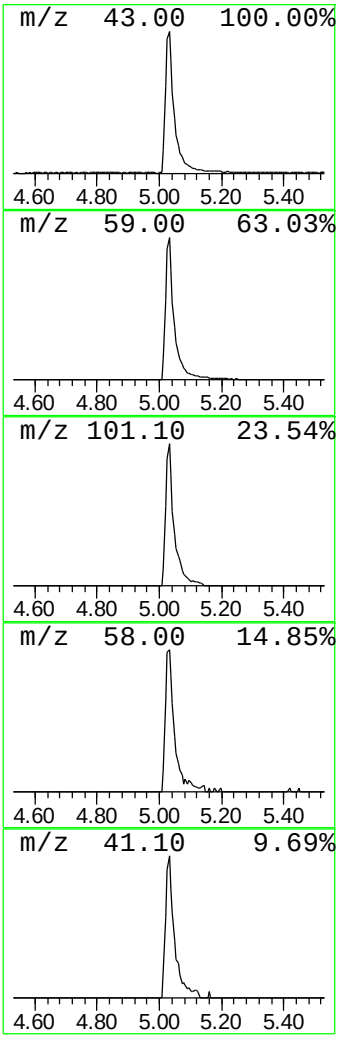
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	14.09 ng	397797	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 10 May 2017 1:28
Operator : SJ/MA
Sample : I3027-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4-5-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
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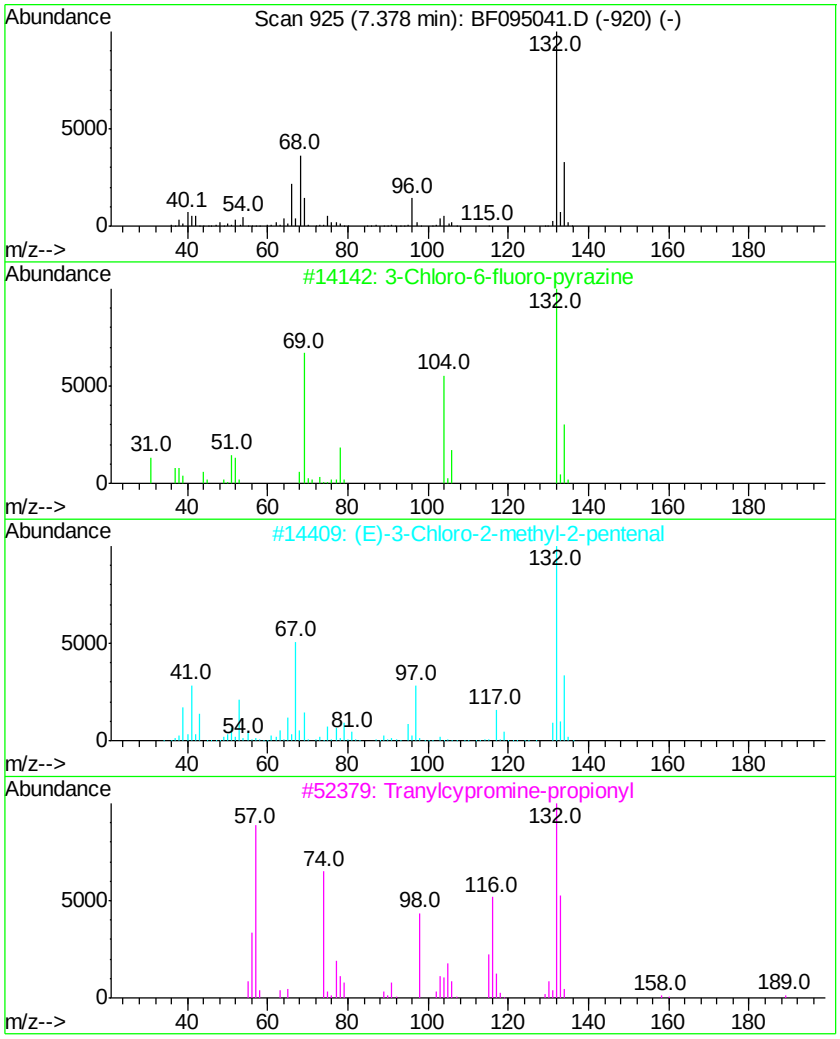
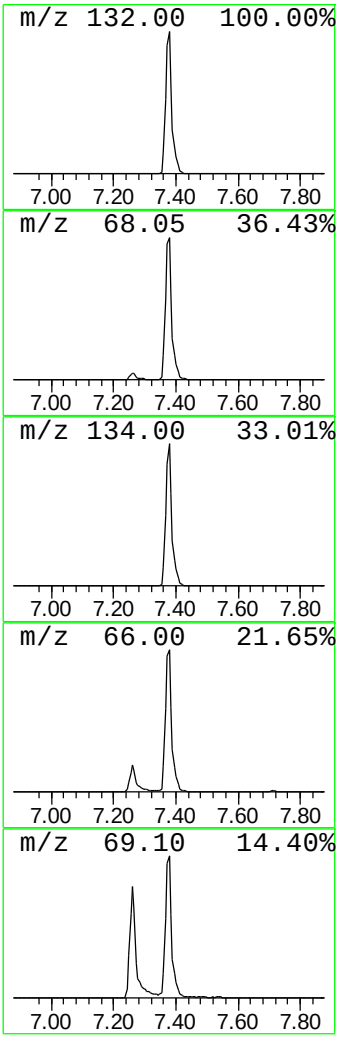
Peak Number 3 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	85.08 ng	2401940	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Misc :
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Instrument : BNA_F
ClientSampleId : TP-4-5-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
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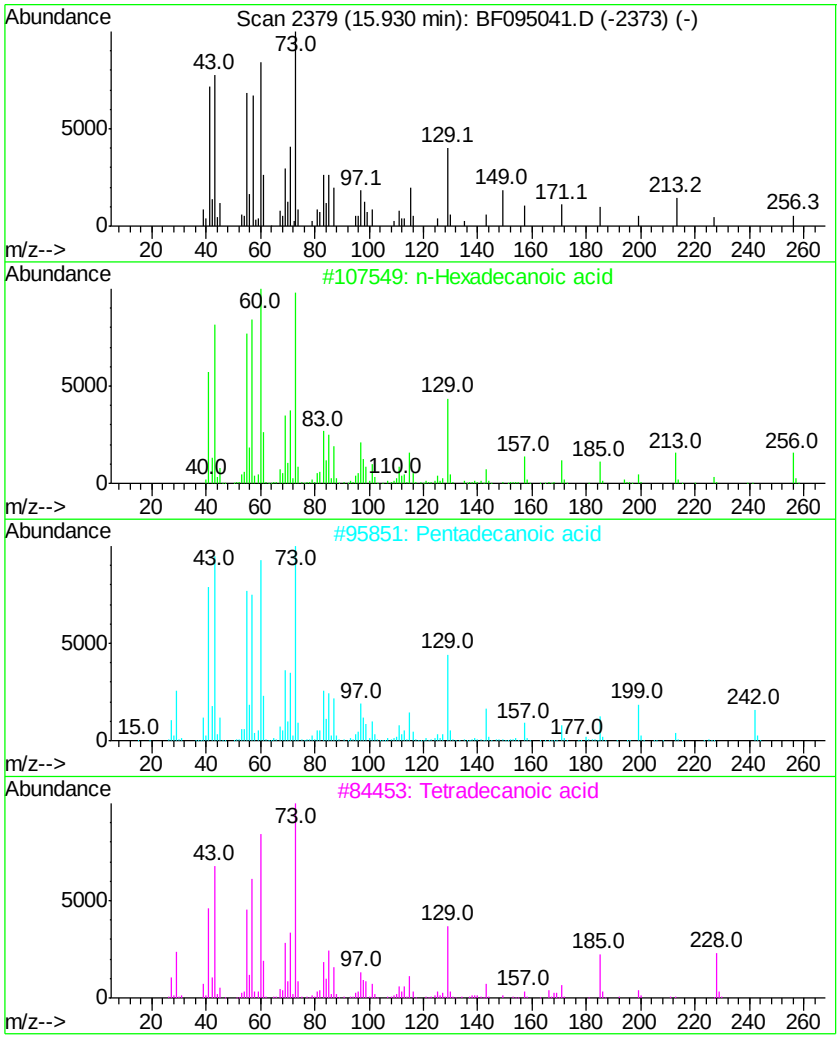
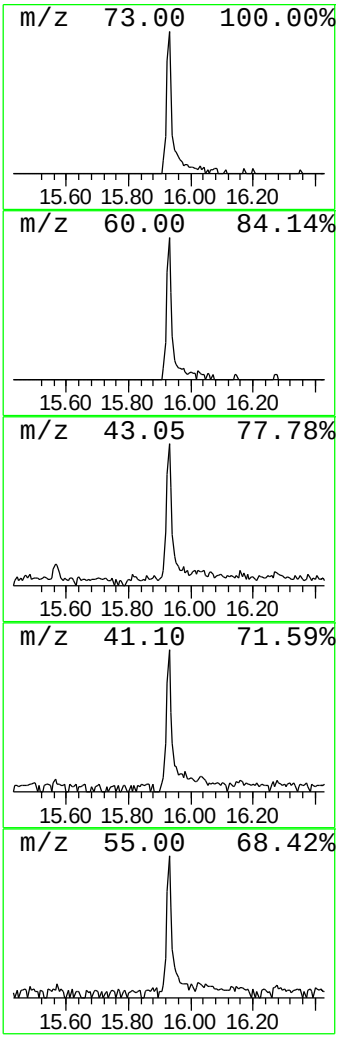
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	4.16 ng	155863	Phenanthrene-d10	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Tetradecane	198	C14H30	000629-59-4	11





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TP-4-5-6-COMP

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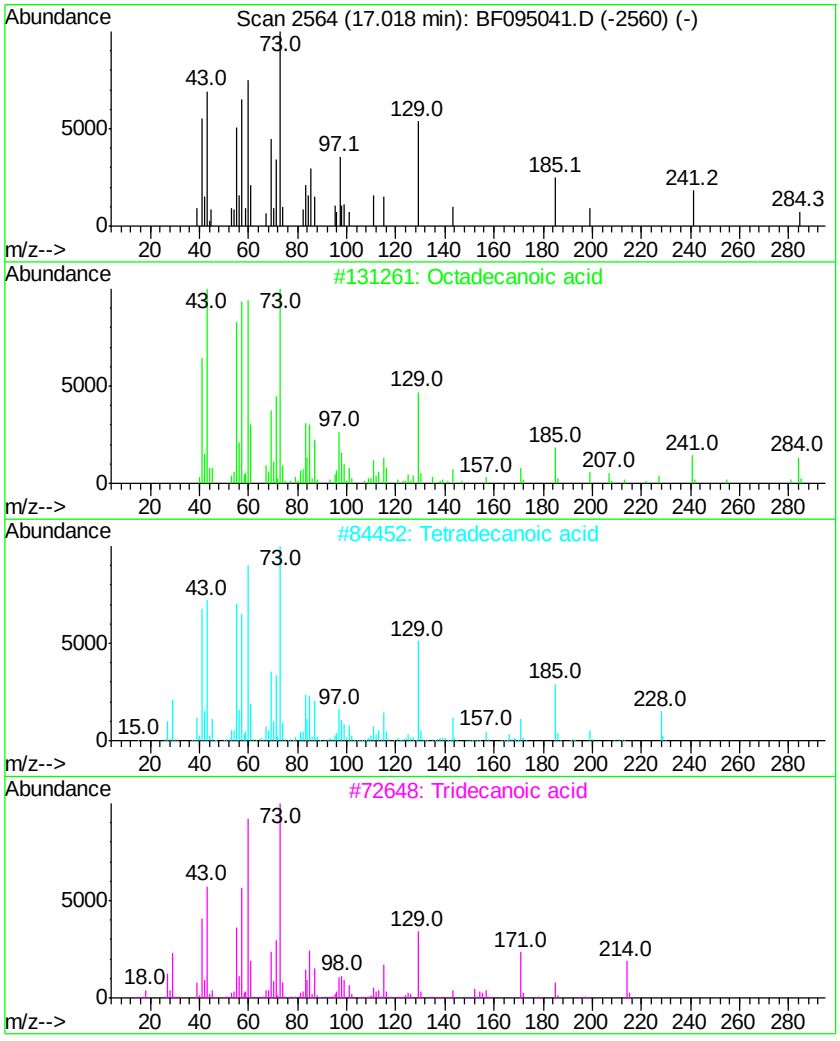
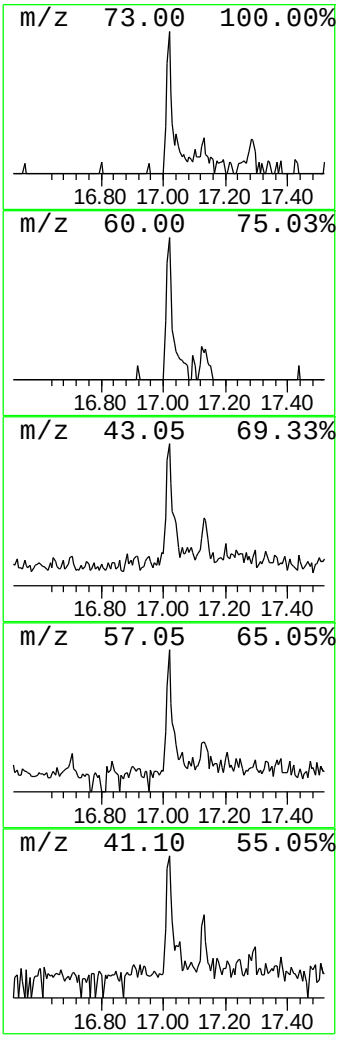
Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	2.19 ng	60650	Chrysene-d12	18.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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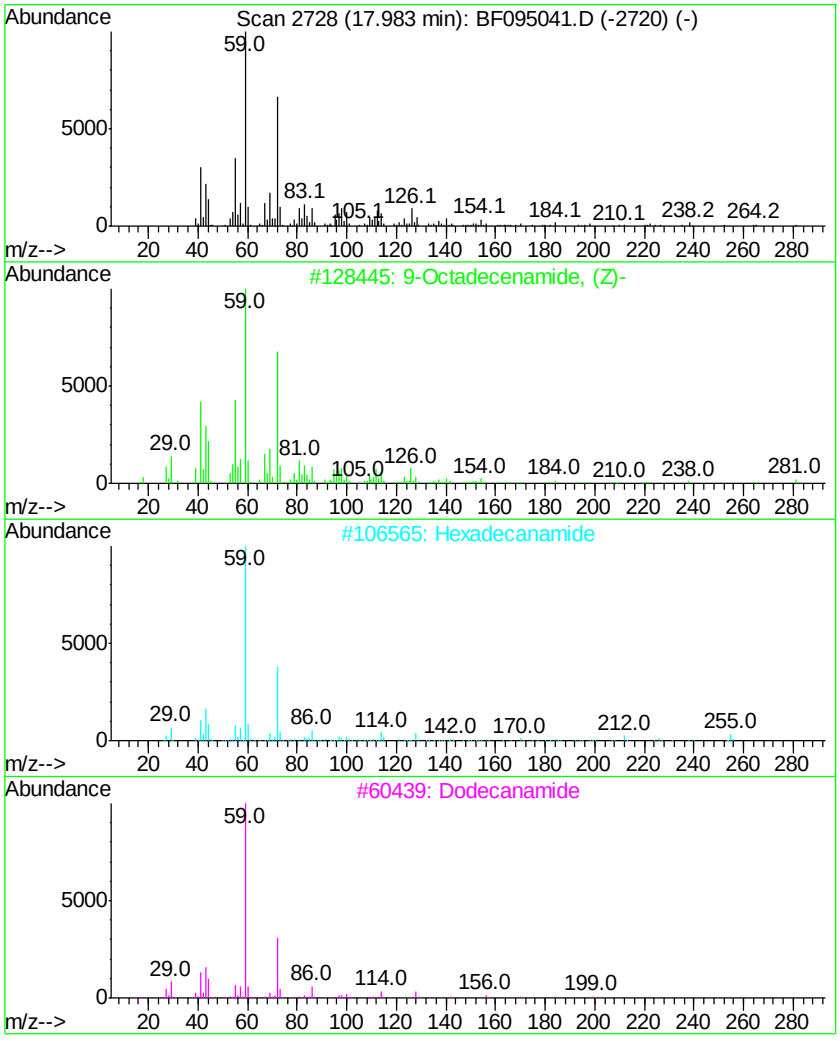
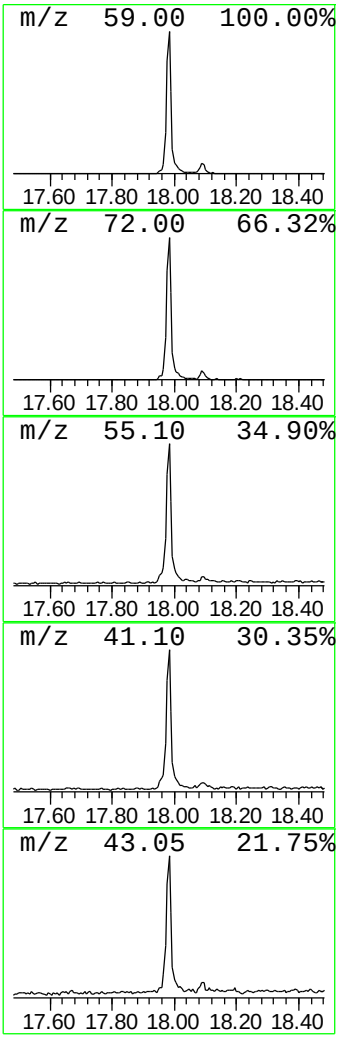
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	22.50 ng	623110	Chrysene-d12	18.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Hexadecanamide	255	C16H33NO	000629-54-9	78
3	Dodecanamide	199	C12H25NO	001120-16-7	59
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
5	Octanamide	143	C8H17NO	000629-01-6	56





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Instrument : BNA_F
ClientSampleId : TP-4-5-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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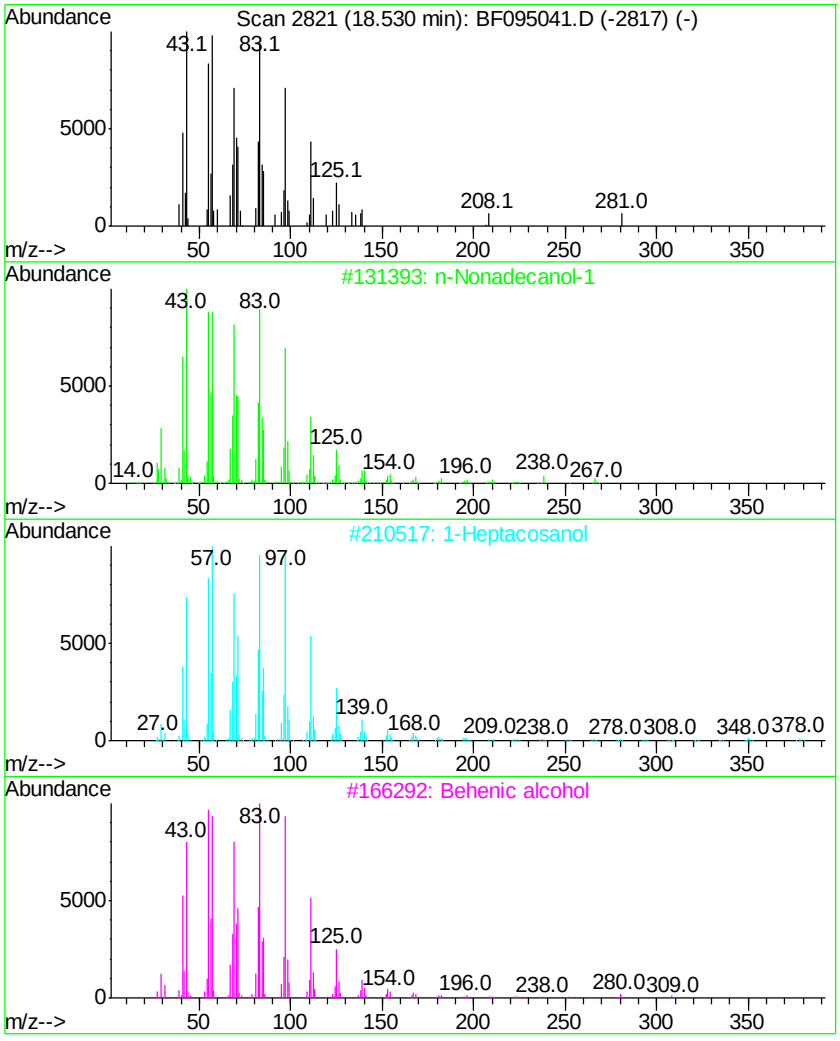
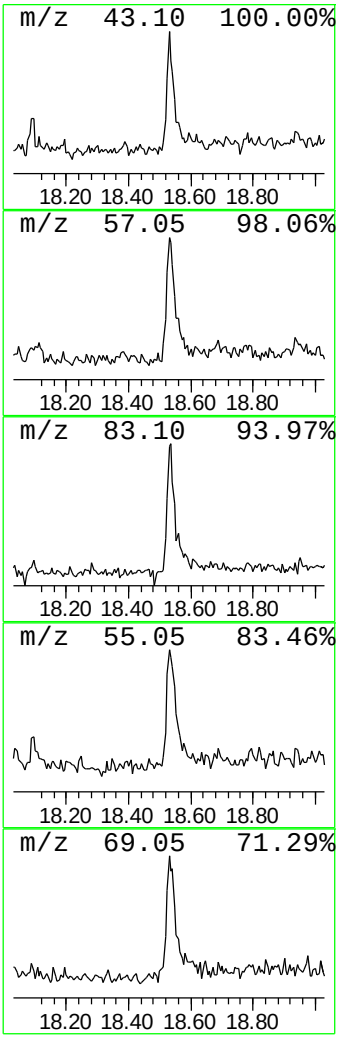
Peak Number 8 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.53	4.30 ng	119194	Chrysene-d12	18.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	93
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5	Isoheptadecanol	256	C17H36O	057289-07-3	90





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.11	2.9	ng	81933	1	7.71	564633	20.0
2-Pentanone, 4-hy...	5.03	14.1	ng	397797	1	7.71	564633	20.0
unknown7.38	7.38	85.1	ng	2401940	1	7.71	564633	20.0
n-Hexadecanoic acid	15.93	4.2	ng	155863	4	14.96	750064	20.0
Octadecanoic acid	17.02	2.2	ng	60650	5	18.63	553894	20.0
9-Octadecenamide,...	17.98	22.5	ng	623110	5	18.63	553894	20.0
n-Nonadecanol-1	18.53	4.3	ng	119194	5	18.63	553894	20.0