LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041425\
Data File : BM049919.D
Acq On : 14 Apr 2025 18:27
Operator : RC/JU
Sample : Q1779-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-23

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_M\Methods\8270-BM040825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049919.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	318	323	332	rBV	1613049	2234286	11.30%	2.129%
2	5.357	396	403	411	rBV	6434557	9174850	46.39%	8.743%
3	5.963	500	506	517	rVB	334573	501641	2.54%	0.478%
4	6.951	662	674	689	rBV	5758575	9505574	48.06%	9.058%
5	7.769	805	813	821	rBV	1641199	2456739	12.42%	2.341%
6	8.145	869	877	885	rVB	309281	502561	2.54%	0.479%
7	8.928	1003	1010	1021	rVB	3559833	5788997	29.27%	5.517%
8	10.563	1280	1288	1302	rBV	1917455	3181686	16.09%	3.032%
9	13.033	1700	1708	1719	rBV	10168021	14243190	72.01%	13.573%
10	14.410	1936	1942	1950	rBV	2870328	4261348	21.54%	4.061%
11	15.768	2168	2173	2180	rBV	810430	1142719	5.78%	1.089%
12	15.904	2189	2196	2206	rBV	8864190	11709349	59.20%	11.159%
13	17.157	2403	2409	2415	rBV	3624289	4841342	24.48%	4.614%
14	18.057	2557	2562	2584	rBV	1102853	2227048	11.26%	2.122%
15	19.215	2755	2759	2762	rBV	152124	197946	1.00%	0.189%
16	19.339	2775	2780	2791	rBV	413905	863807	4.37%	0.823%
17	19.780	2850	2855	2866	rBV	16642872	19779724	100.00%	18.849%
18	21.080	3072	3076	3087	rBV	565439	1266476	6.40%	1.207%
19	21.392	3124	3129	3142	rVB	3579312	5130583	25.94%	4.889%
20	22.192	3260	3265	3277	rVB	665647	1575792	7.97%	1.502%
21	24.386	3631	3638	3649	rVB	1787695	4350845	22.00%	4.146%

Sum of corrected areas: 104936503

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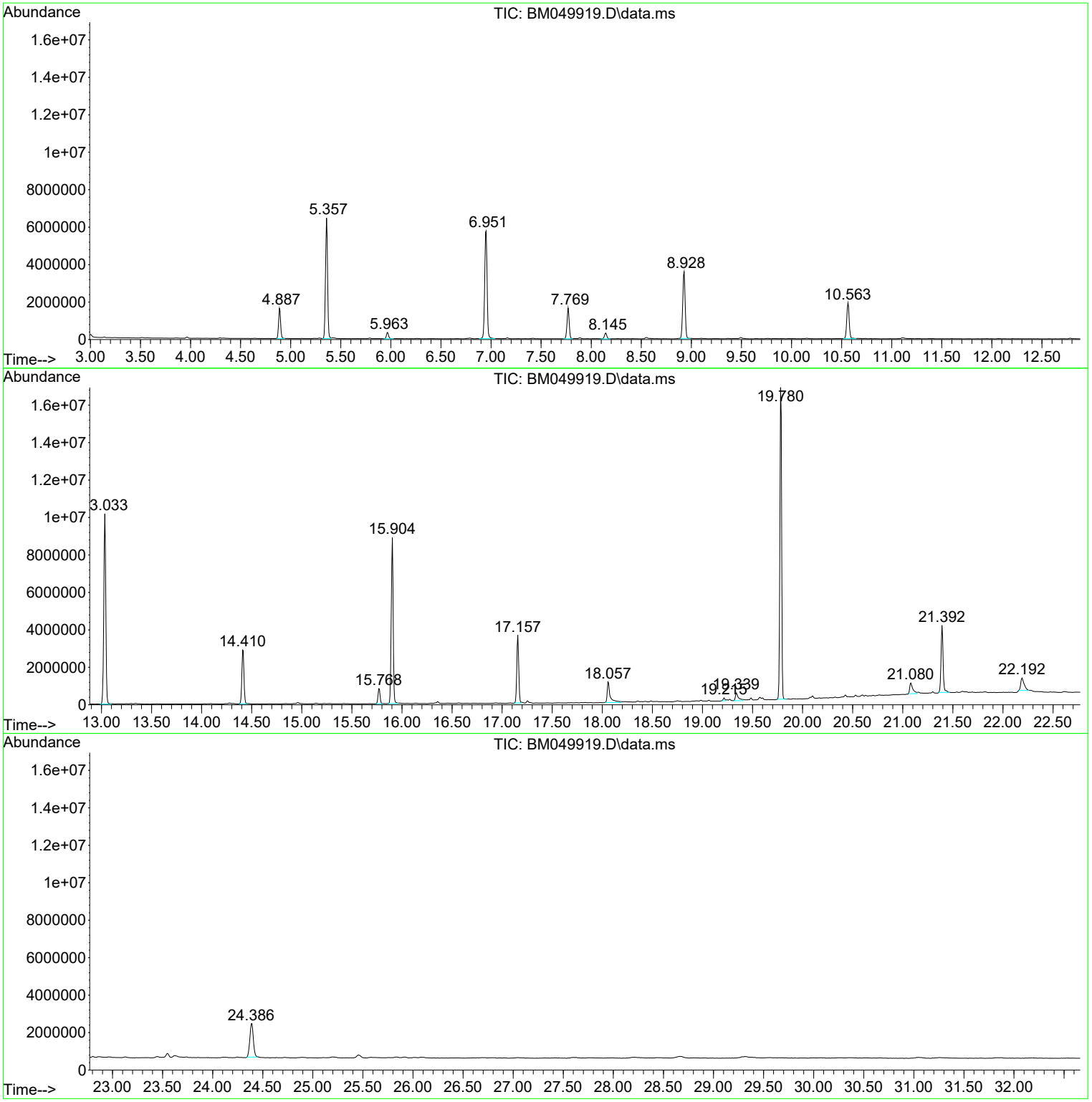
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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_M\Data\BM041425\
Data File : BM049919.D
Acq On : 14 Apr 2025 18:27
Operator : RC/JU
Sample : Q1779-05
Misc :
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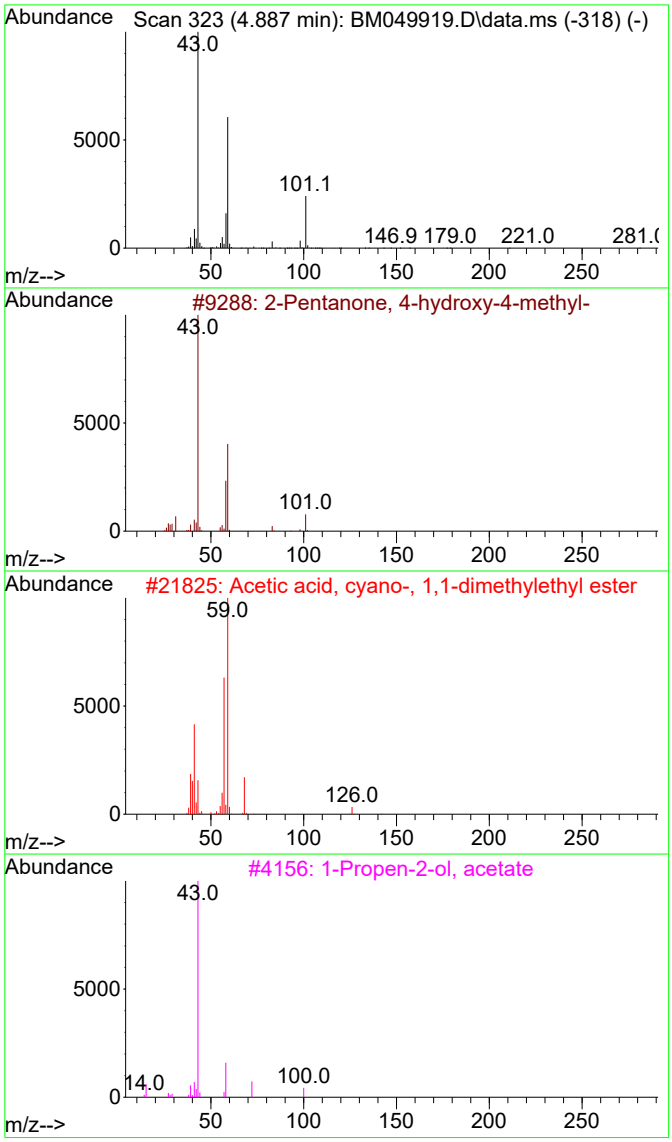
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

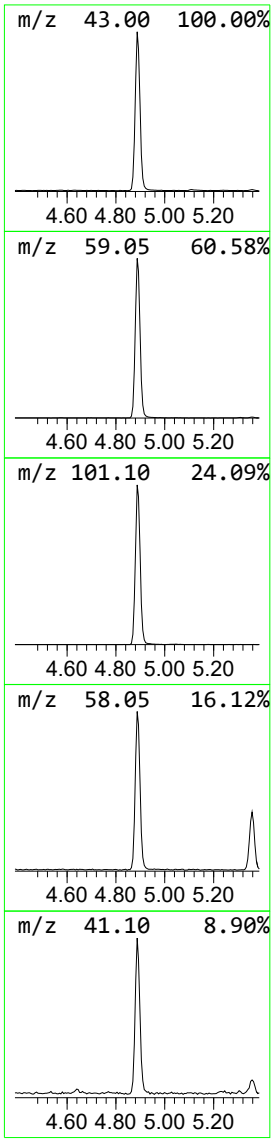
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	18.19 ng	2234290	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
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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Data File : BM049919.D
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Operator : RC/JU
Sample : Q1779-05
Misc :
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Instrument :
BNA_M
ClientSampleId :
TP-23

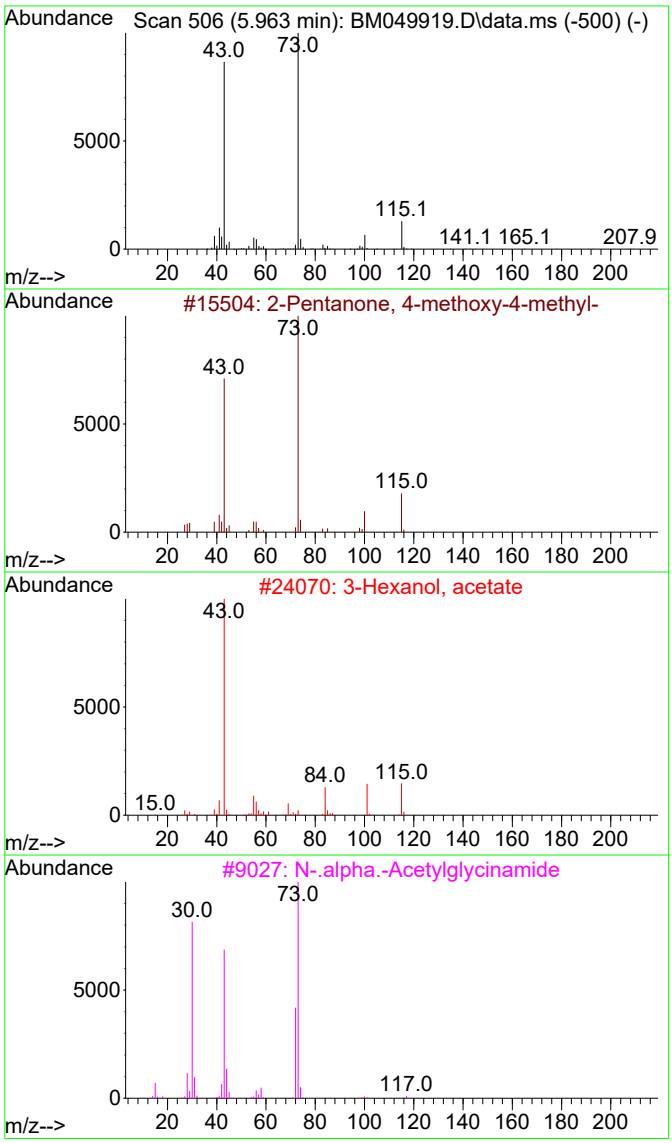
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

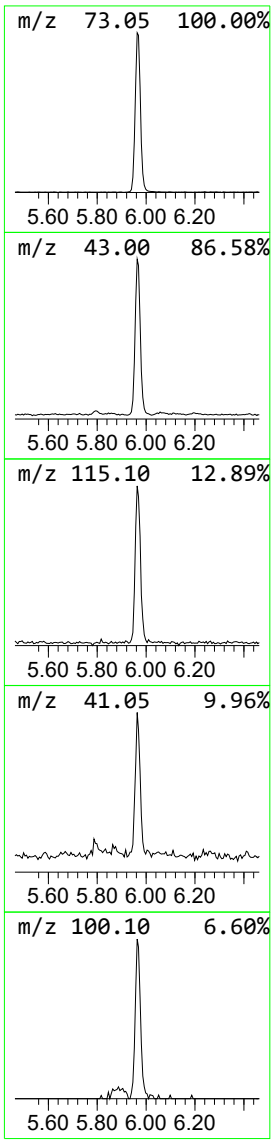
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.963	4.08 ng	501641	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3-Hexanol, acetate	144	C8H16O2	040780-64-1	32
3	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4	3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
5	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23





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Data File : BM049919.D
Acq On : 14 Apr 2025 18:27
Operator : RC/JU
Sample : Q1779-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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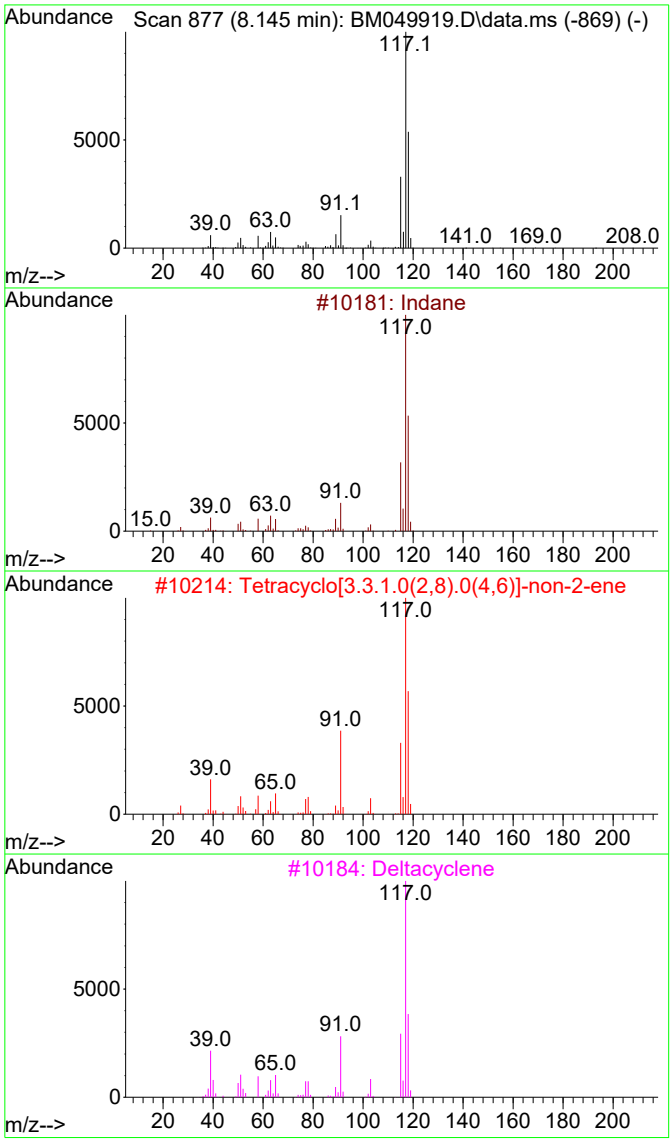
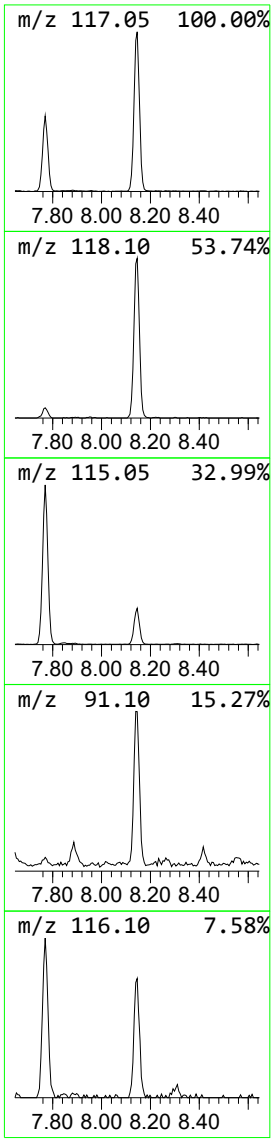
****

Peak Number 3 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.145	4.09 ng	502561	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
3	Deltacyclene	118	C9H10	007785-10-6	72
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59





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Data File : BM049919.D
Acq On : 14 Apr 2025 18:27
Operator : RC/JU
Sample : Q1779-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

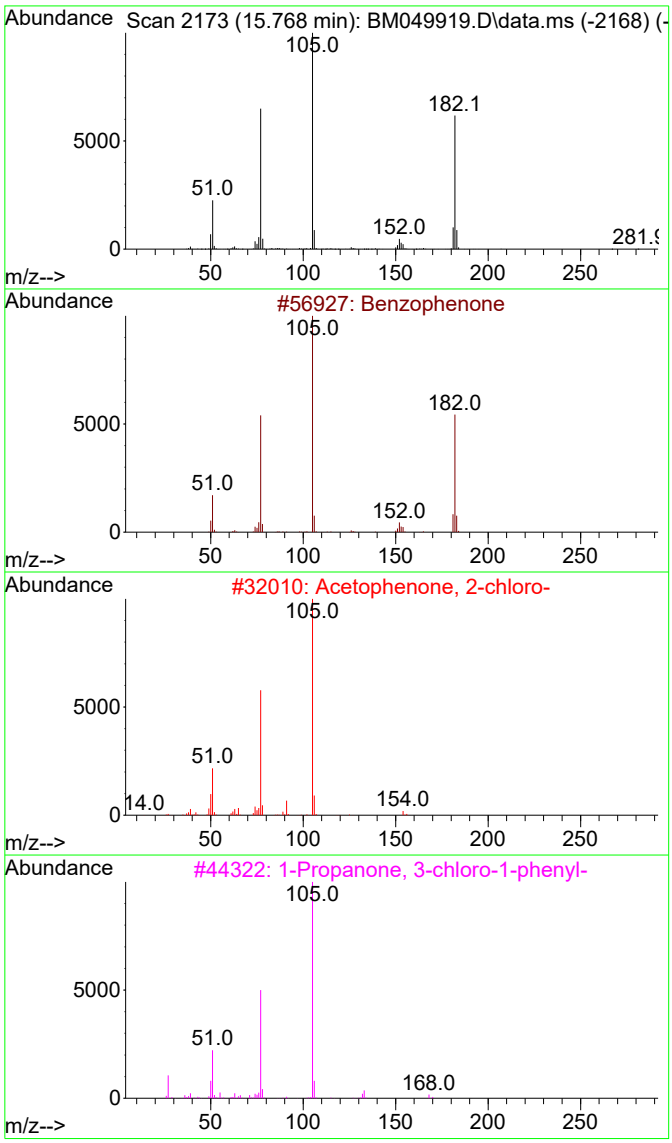
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

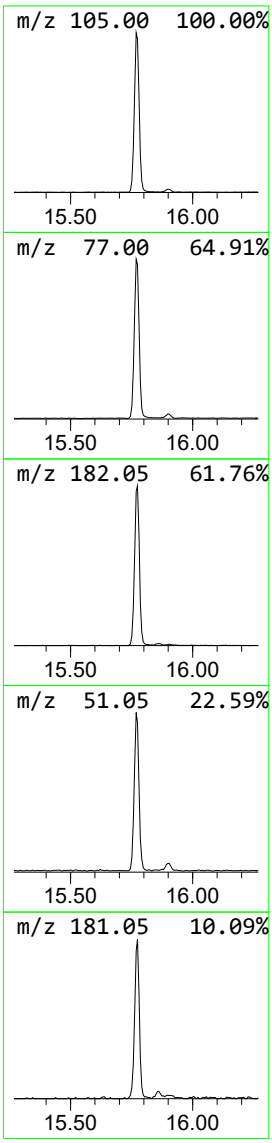
****

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.769	5.36 ng	1142720	Acenaphthene-d10	14.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
5	Azobenzene	182	C12H10N2	000103-33-3	47





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Acq On : 14 Apr 2025 18:27
Operator : RC/JU
Sample : Q1779-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

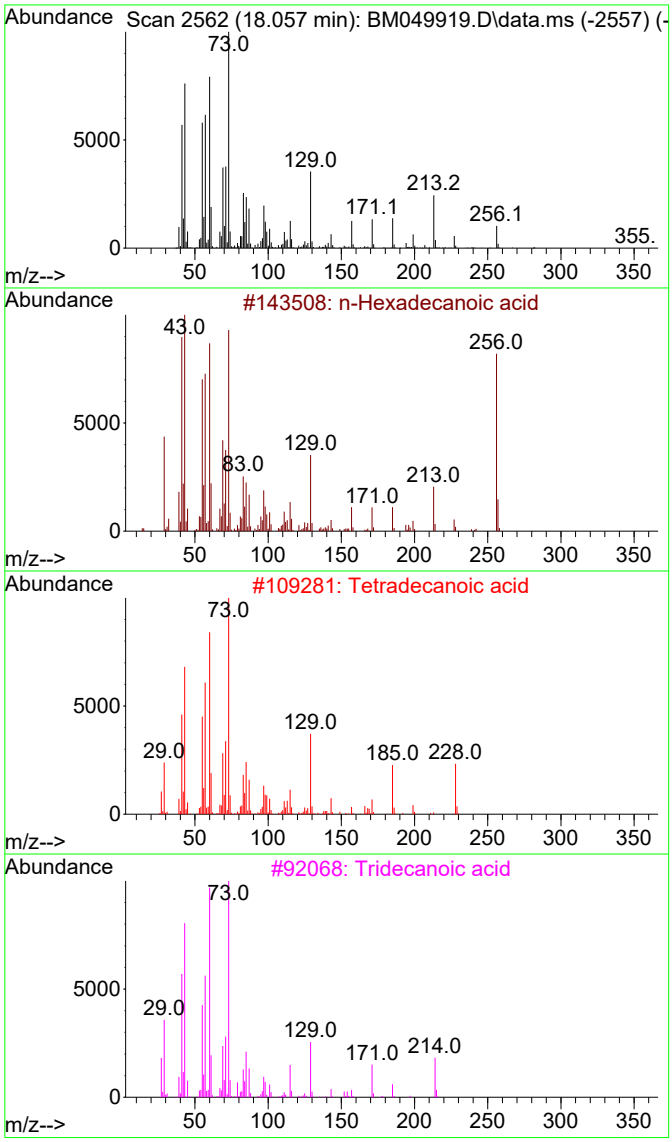
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

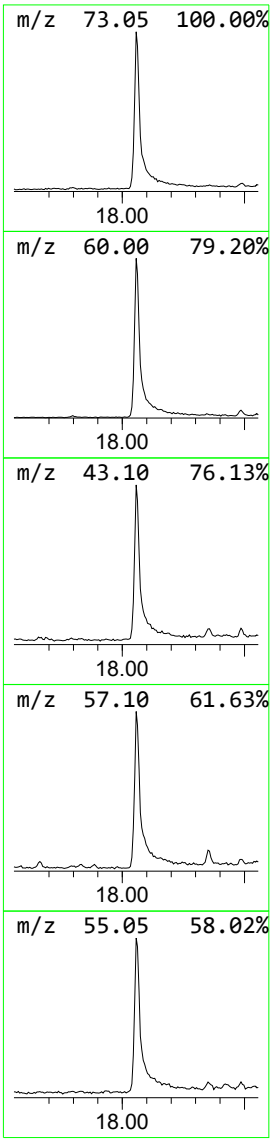
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.057	9.20 ng	2227050	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	53





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
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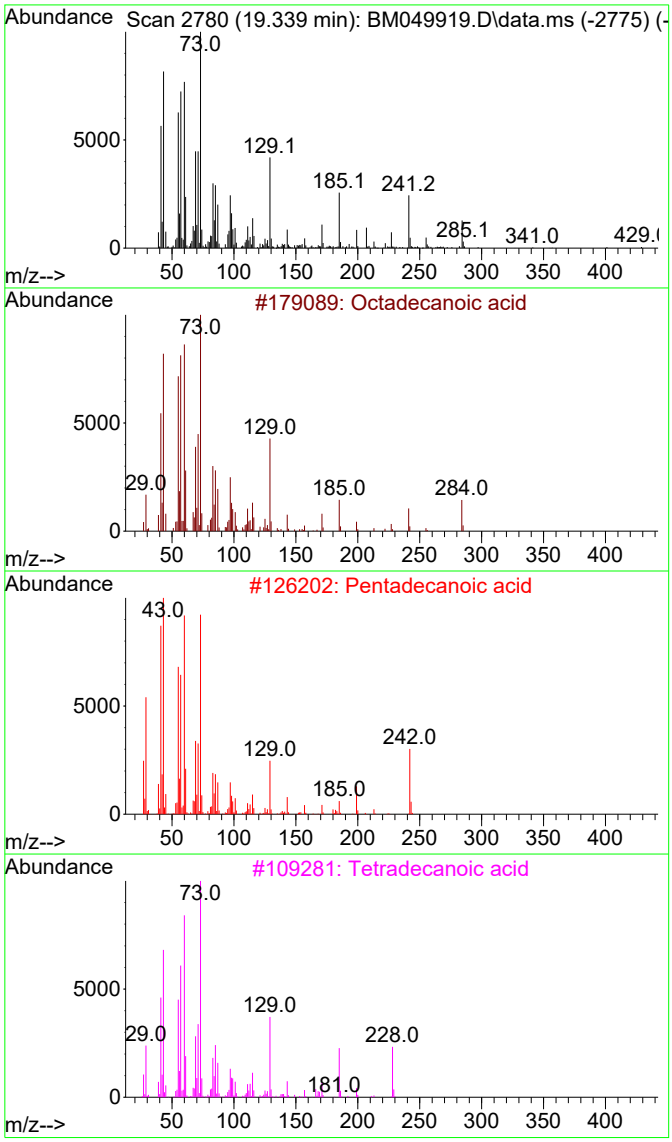
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

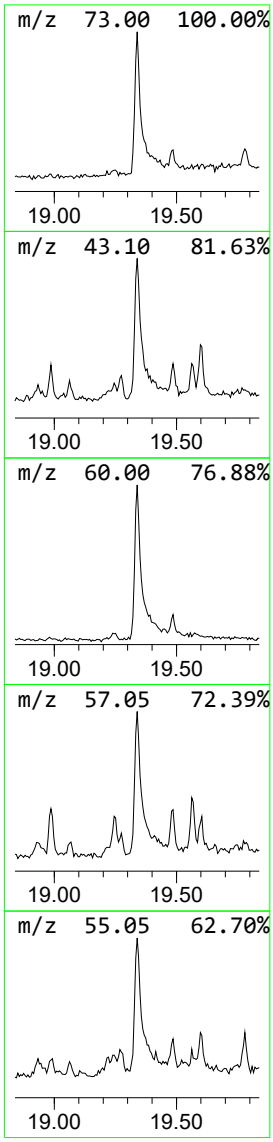
****

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	3.37 ng	863807	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64





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Sample : Q1779-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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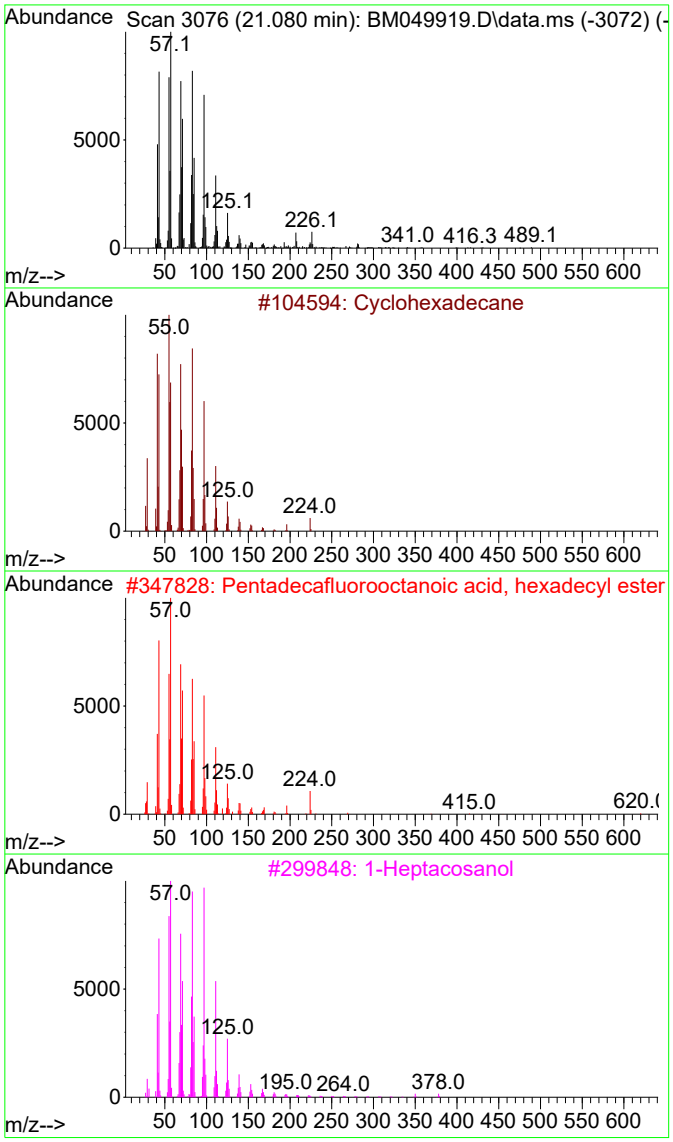
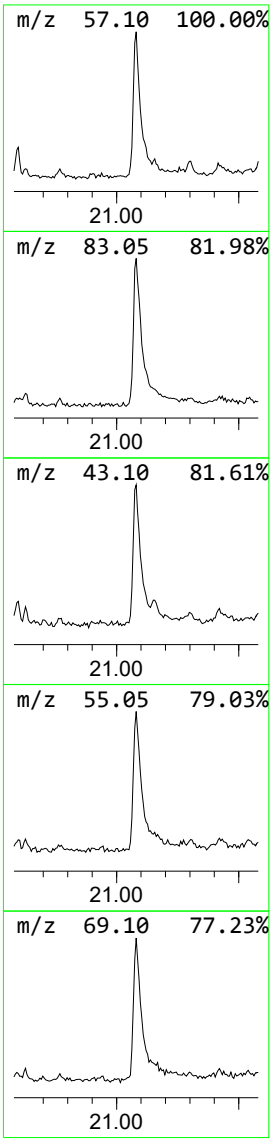
****

Peak Number 7 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	4.94 ng	1266480	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	92





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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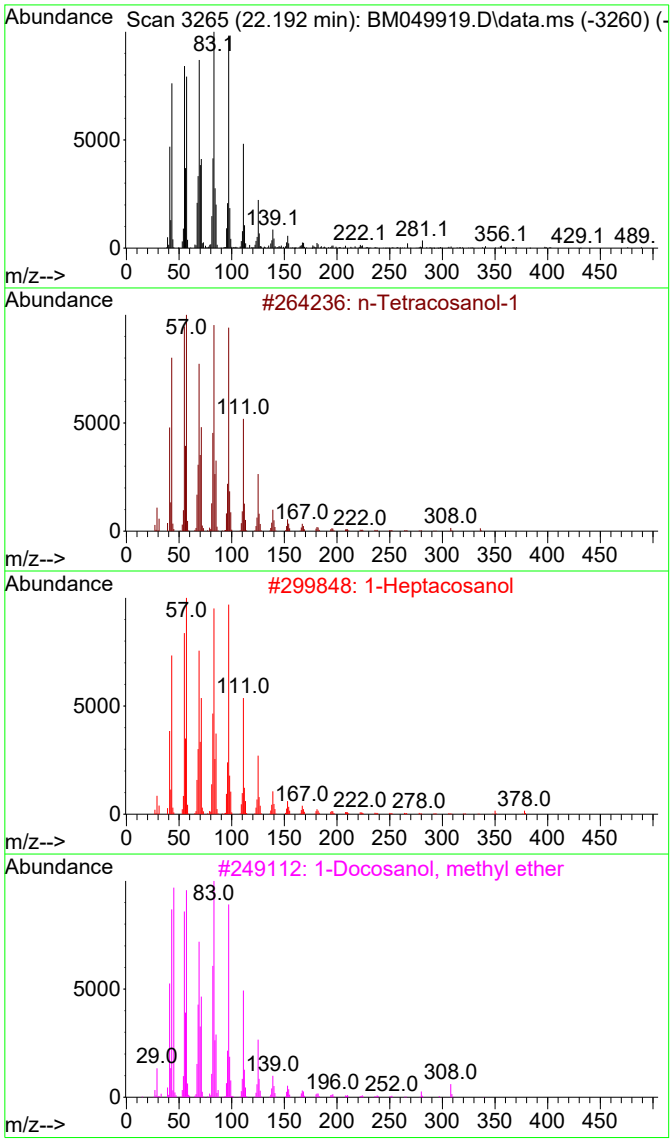
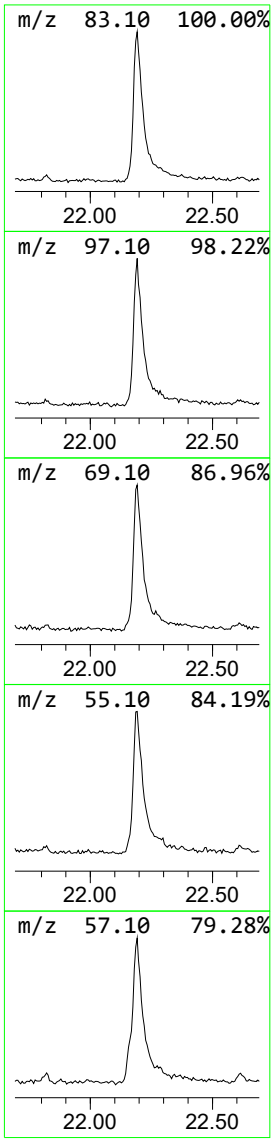
****

Peak Number 8 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.192	6.14 ng	1575790	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	1-Hexadecanol	242	C16H34O	036653-82-4	91





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-...	4.887	18.2	ng	2234290	1	7.769	2456740	20.0
2-Pentanone, 4-...	5.963	4.1	ng	501641	1	7.769	2456740	20.0
Indane	8.145	4.1	ng	502561	1	7.769	2456740	20.0
Benzophenone	15.769	5.4	ng	1142720	3	14.416	4261350	20.0
n-Hexadecanoic ...	18.057	9.2	ng	2227050	4	17.157	4841340	20.0
Octadecanoic acid	19.339	3.4	ng	863807	5	21.392	5130580	20.0
Cyclohexadecane	21.080	4.9	ng	1266480	5	21.392	5130580	20.0
n-Tetracosanol-1	22.192	6.1	ng	1575790	5	21.392	5130580	20.0