LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047561.D
Acq On : 18 Sep 2024 18:26
Operator : RC/JU
Sample : P4088-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-07

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-BM091424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047561.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	313	319	328	rVB	254063	367736	4.97%	0.748%
2	5.422	390	397	409	rBV	3781288	5438978	73.58%	11.070%
3	7.010	658	667	677	rBV	3722084	5715923	77.33%	11.633%
4	7.851	803	810	818	rBV	1074062	1654976	22.39%	3.368%
5	9.004	997	1006	1017	rBV	2102976	3413506	46.18%	6.947%
6	9.569	1097	1102	1109	rVB	49768	77684	1.05%	0.158%
7	10.645	1277	1285	1294	rBV	1281810	2174301	29.42%	4.425%
8	13.110	1696	1704	1717	rBV	4277546	6351049	85.92%	12.926%
9	14.480	1930	1937	1944	rBV	1670036	2372218	32.09%	4.828%
10	15.833	2161	2167	2175	rBV	1107484	1462992	19.79%	2.978%
11	15.962	2182	2189	2206	rBV	3091602	4200803	56.83%	8.550%
12	16.398	2258	2263	2274	rVB	172690	245311	3.32%	0.499%
13	17.215	2396	2402	2408	rBV	1758294	2459046	33.27%	5.005%
14	18.109	2549	2554	2563	rBV	198541	295142	3.99%	0.601%
15	19.386	2767	2771	2776	rBV3	76308	98257	1.33%	0.200%
16	19.833	2841	2847	2857	rBV	6293436	7391800	100.00%	15.044%
17	21.121	3062	3066	3075	rBV2	205379	374890	5.07%	0.763%
18	21.444	3115	3121	3130	rBV	1637040	2405241	32.54%	4.895%
19	22.244	3253	3257	3266	rVB4	150335	272273	3.68%	0.554%
20	24.474	3628	3636	3647	rBV	943902	2361939	31.95%	4.807%

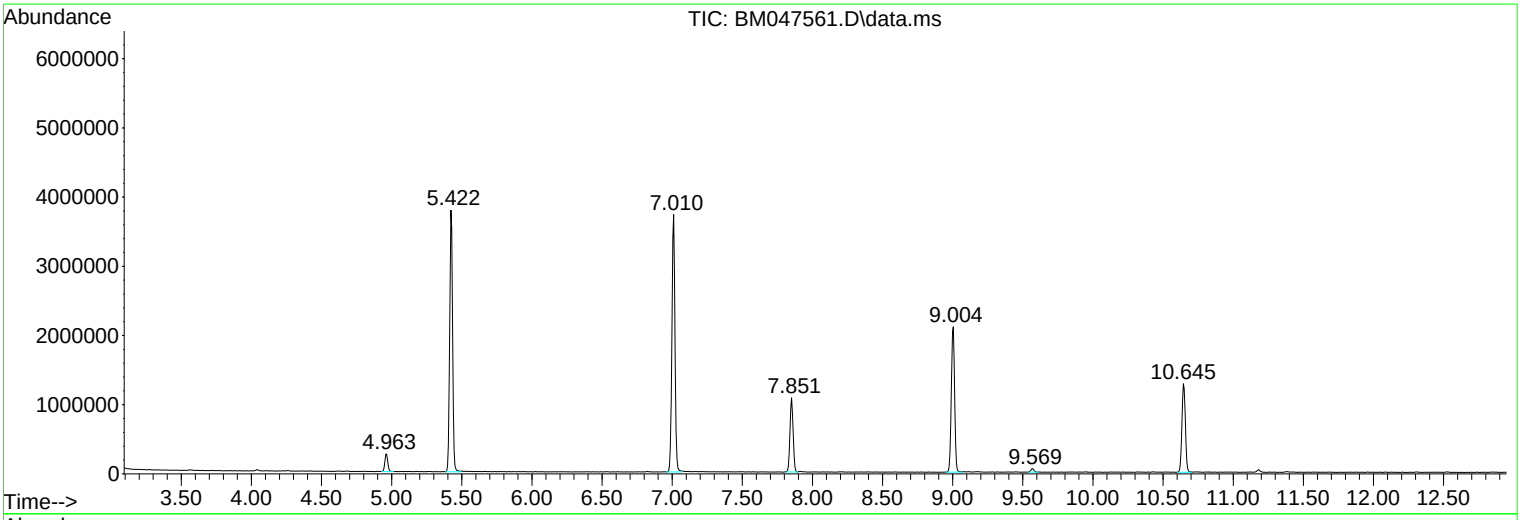
Sum of corrected areas: 49134065

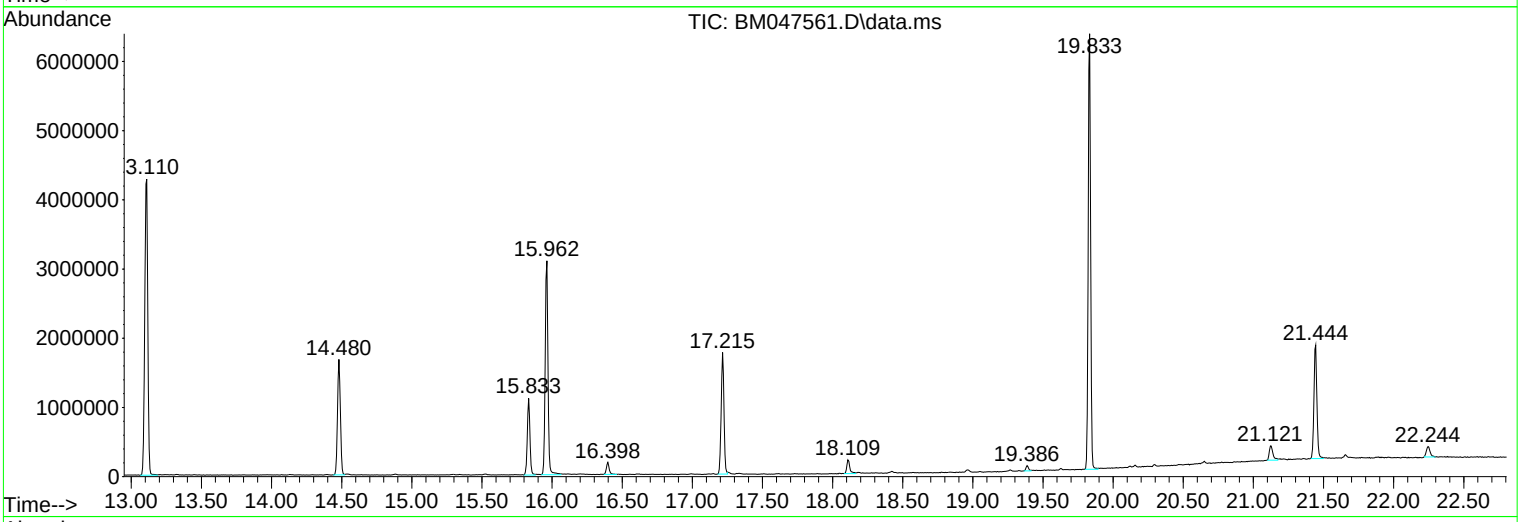
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047561.D
Acq On : 18 Sep 2024 18:26
Operator : RC/JU
Sample : P4088-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

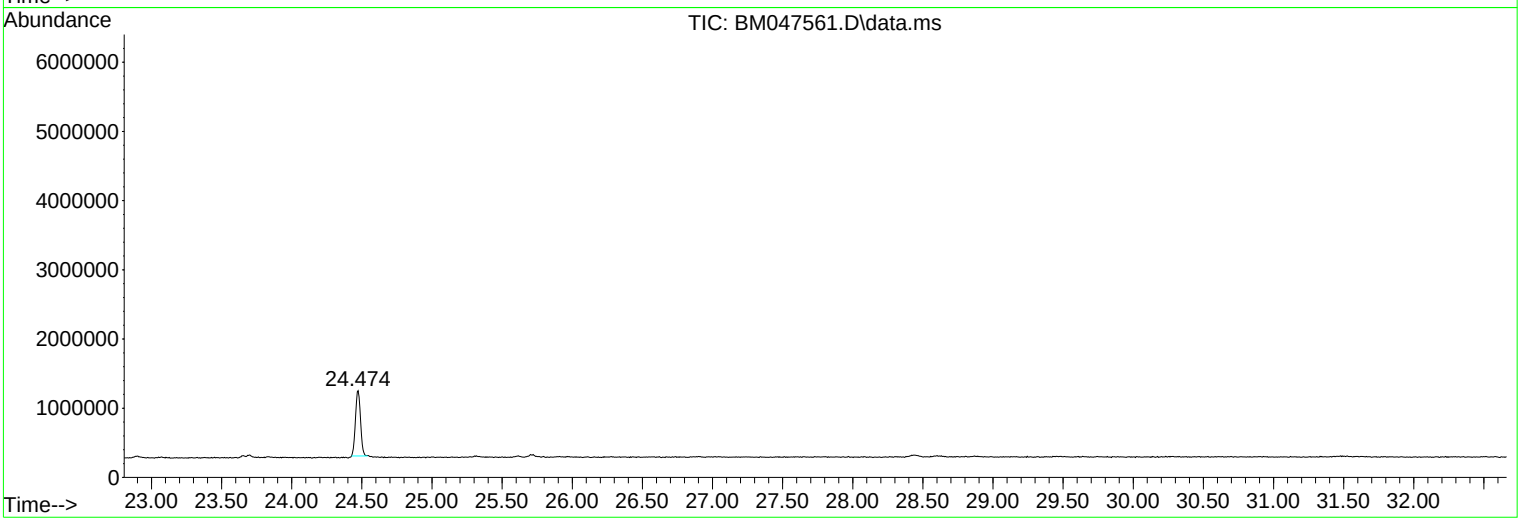
Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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\BM091824\
Data File : BM047561.D
Acq On : 18 Sep 2024 18:26
Operator : RC/JU
Sample : P4088-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-07

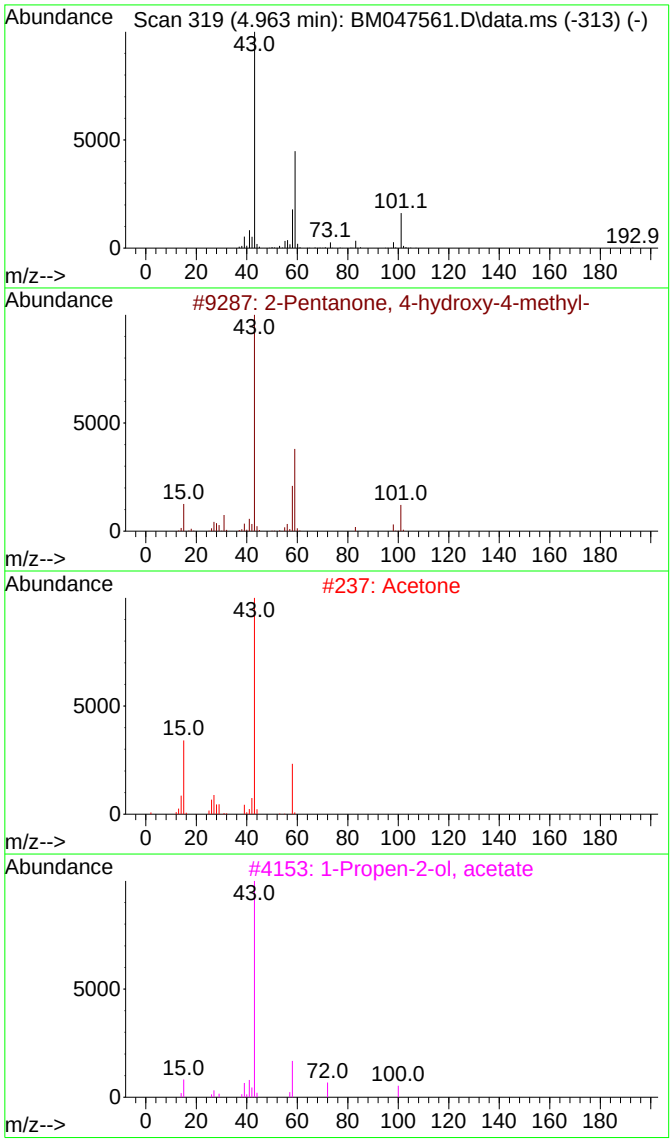
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

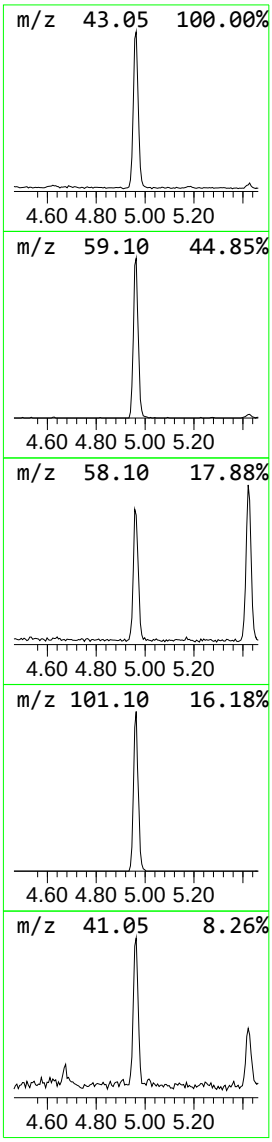
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	4.44 ng	367736	1,4-Dichlorobenzene-d4	7.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	Acetone	58	C3H6O	000067-64-1	12
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047561.D
Acq On : 18 Sep 2024 18:26
Operator : RC/JU
Sample : P4088-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

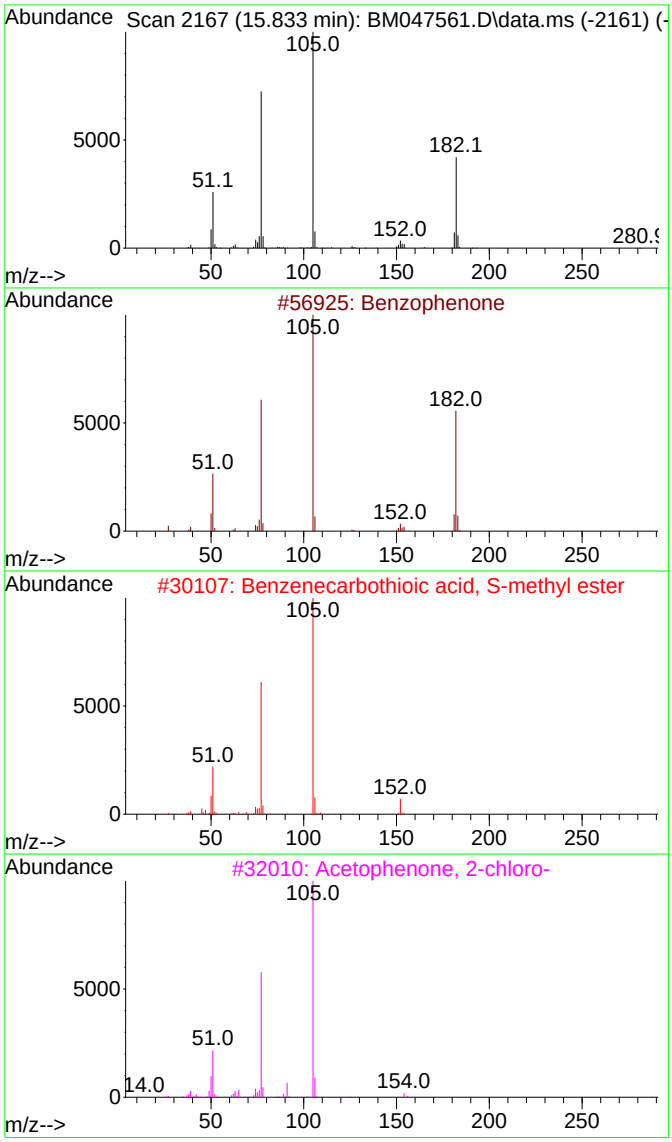
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

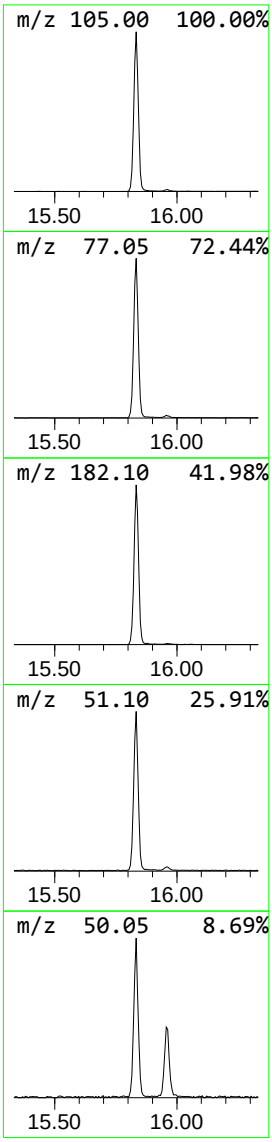
****

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.833	12.33 ng	1462990	Acenaphthene-d10	14.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47
5	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047561.D
Acq On : 18 Sep 2024 18:26
Operator : RC/JU
Sample : P4088-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

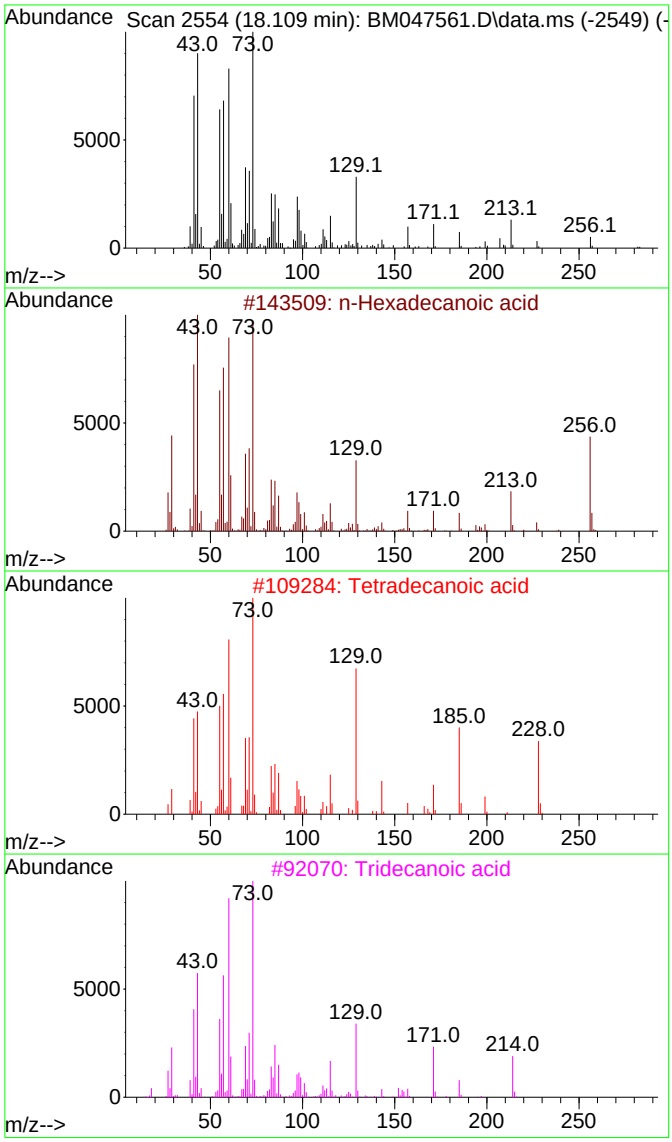
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

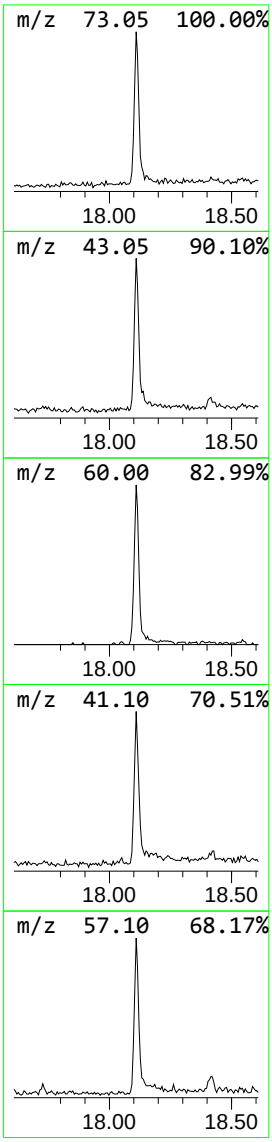
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.109	2.40 ng	295142	Phenanthrene-d10	17.215

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	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047561.D
Acq On : 18 Sep 2024 18:26
Operator : RC/JU
Sample : P4088-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

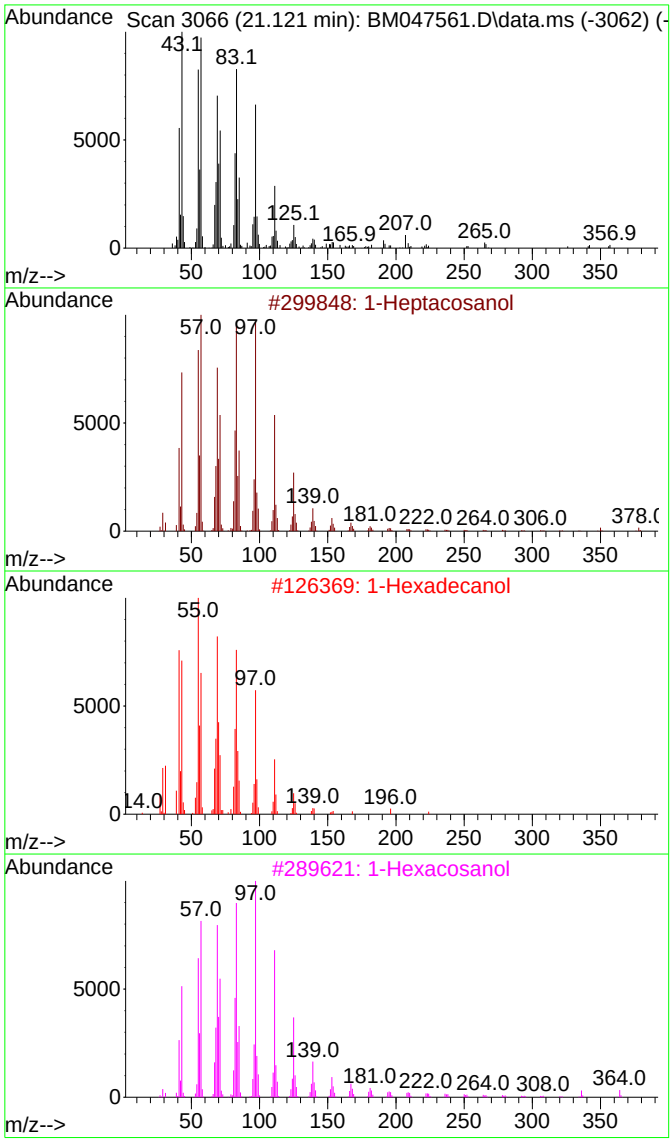
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

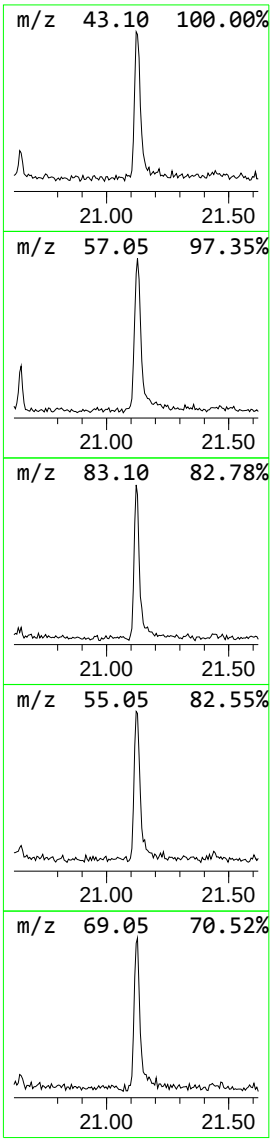
****

Peak Number 4 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	3.12 ng	374890	Chrysene-d12	21.444

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	1-Hexadecanol	242	C16H34O	036653-82-4	93
3	1-Hexacosanol	382	C26H54O	000506-52-5	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5	1-Docosene	308	C22H44	001599-67-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047561.D
Acq On : 18 Sep 2024 18:26
Operator : RC/JU
Sample : P4088-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

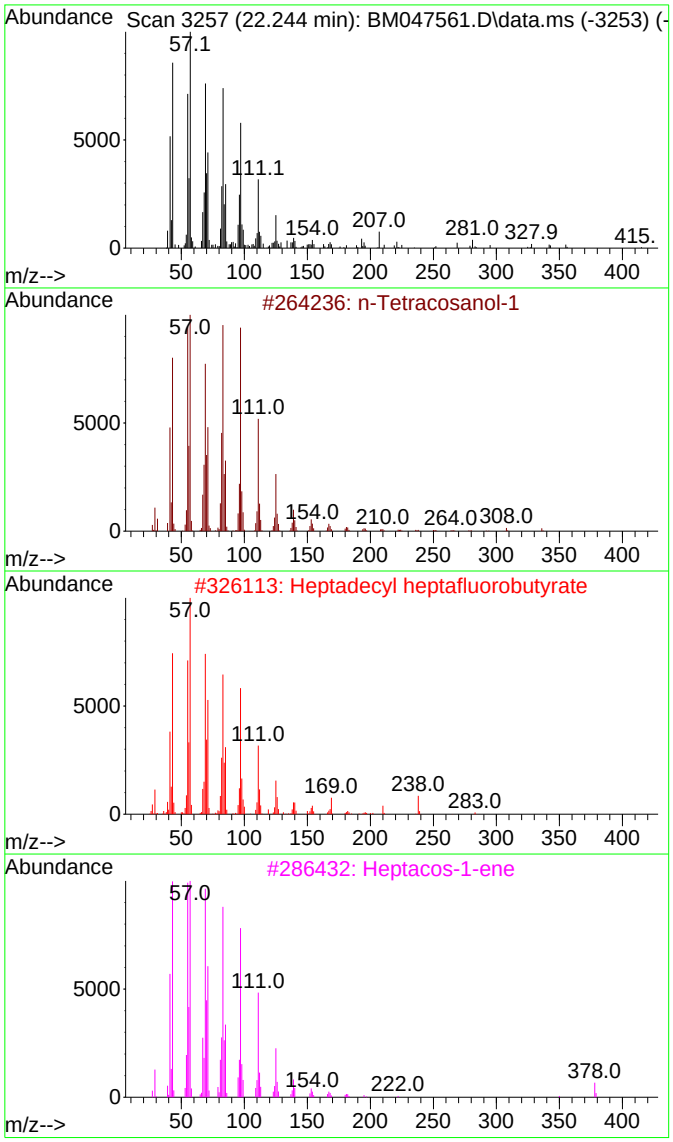
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

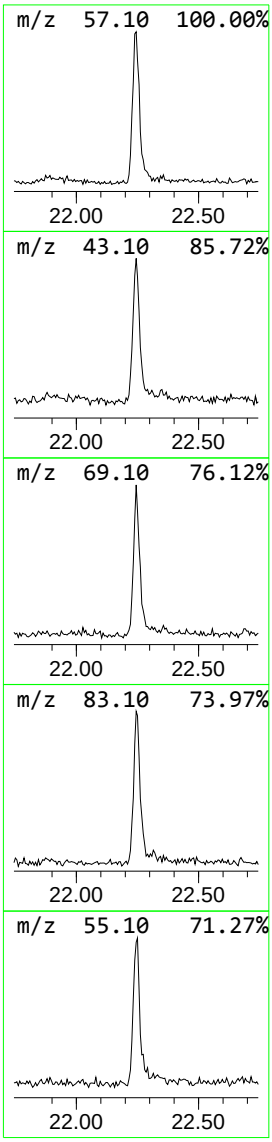
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.244	2.26 ng	272273	Chrysene-d12	21.444

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Heptacos-1-ene	378	C27H54	015306-27-1	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	Octacosanol	410	C28H58O	000557-61-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047561.D
Acq On : 18 Sep 2024 18:26
Operator : RC/JU
Sample : P4088-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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
2-Pentanone, 4-...	4.963	4.4	ng	367736	1	7.851	1654980	20.0
Benzophenone	15.833	12.3	ng	1462990	3	14.480	2372220	20.0
n-Hexadecanoic ...	18.109	2.4	ng	295142	4	17.215	2459050	20.0
1-Heptacosanol	21.121	3.1	ng	374890	5	21.444	2405240	20.0
n-Tetracosanol-1	22.244	2.3	ng	272273	5	21.444	2405240	20.0