LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

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-BM030823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039151.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	290	298	304	rBV	771959	1107344	8.41%	1.650%
2	5.505	371	377	385	rVB	2568480	3614490	27.44%	5.386%
3	7.110	643	650	666	rVB	1450705	2312651	17.56%	3.446%
4	7.946	782	792	800	rBV	834801	1340346	10.18%	1.997%
5	9.116	984	991	1007	rBV	3066435	5061057	38.42%	7.541%
6	10.757	1263	1270	1278	rBV	1041085	1777613	13.50%	2.649%
7	12.275	1523	1528	1537	rBV	78589	150656	1.14%	0.224%
8	13.216	1678	1688	1695	rBV	7382103	10730266	81.46%	15.988%
9	14.404	1886	1890	1894	rBV3	132904	197469	1.50%	0.294%
10	14.592	1915	1922	1928	rBV	1560086	2336582	17.74%	3.481%
11	14.810	1956	1959	1966	rBV7	59124	136330	1.04%	0.203%
12	15.192	2021	2024	2029	rBV4	93198	174800	1.33%	0.260%
13	15.239	2029	2032	2036	rVB2	114401	146322	1.11%	0.218%
14	15.551	2081	2085	2093	rVB5	175629	345763	2.63%	0.515%
15	15.686	2104	2108	2115	rVB6	119749	205562	1.56%	0.306%
16	15.904	2142	2145	2148	rBV4	93132	133755	1.02%	0.199%
17	15.951	2148	2153	2158	rVV	1723798	2357917	17.90%	3.513%
18	16.080	2169	2175	2188	rVB	5769910	8451645	64.17%	12.593%
19	16.510	2244	2248	2255	rVB	268626	405648	3.08%	0.604%
20	16.839	2300	2304	2316	rVB	1110243	1494807	11.35%	2.227%
21	17.339	2384	2389	2393	rBV	1701644	2394880	18.18%	3.568%
22	18.233	2537	2541	2551	rBV	1289614	1733828	13.16%	2.583%
23	19.504	2754	2757	2766	rBV	552459	788313	5.98%	1.175%
24	19.957	2829	2834	2840	rBV	10070450	13171650	100.00%	19.626%
25	20.868	2987	2989	2994	rVB	227633	250363	1.90%	0.373%
26	21.221	3045	3049	3055	rBV	687848	864461	6.56%	1.288%
27	21.515	3095	3099	3106	rVB	2082534	2647286	20.10%	3.944%
28	23.939	3506	3511	3519	rVB2	1386801	2782962	21.13%	4.147%

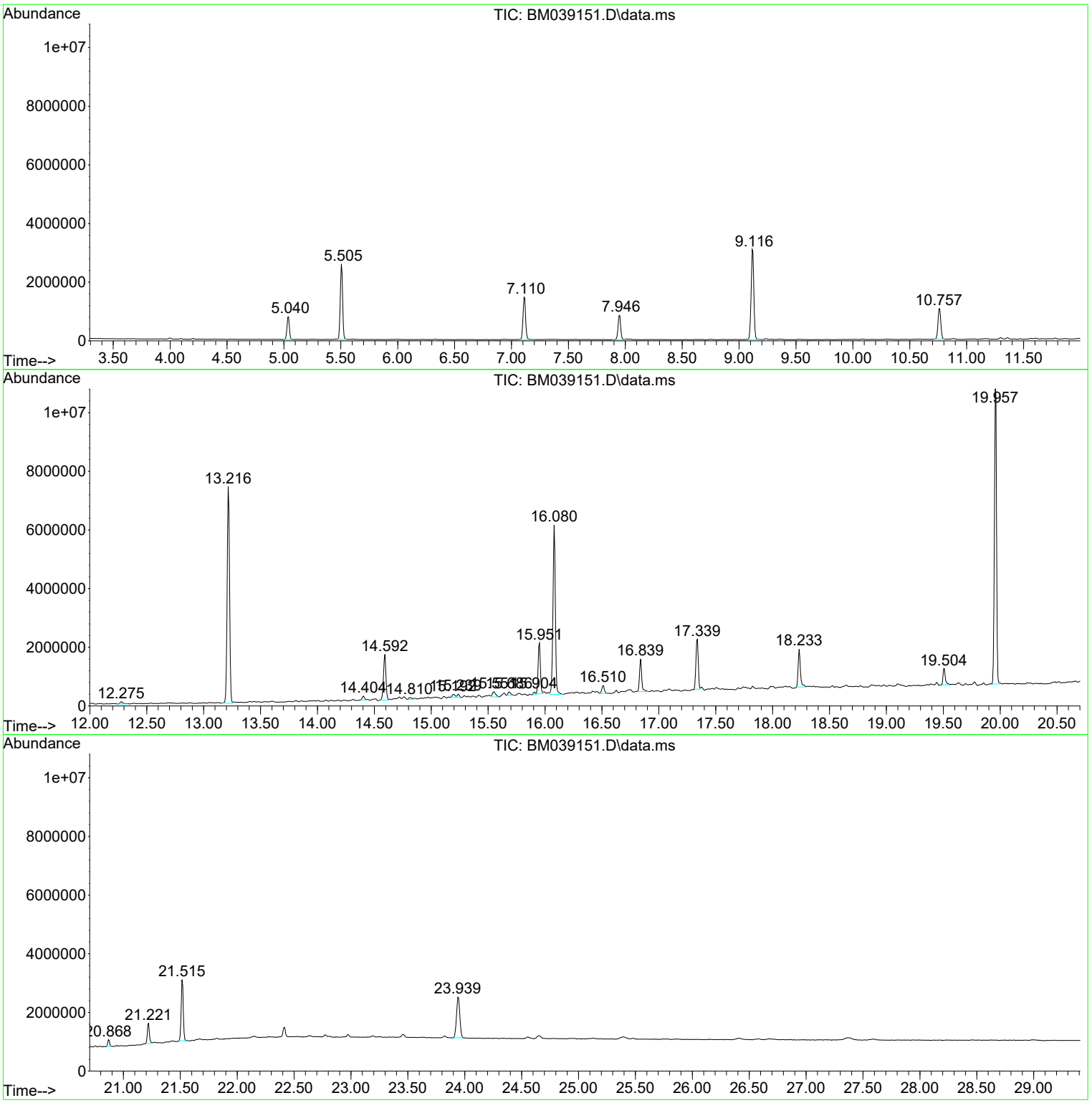
Sum of corrected areas: 67114766

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

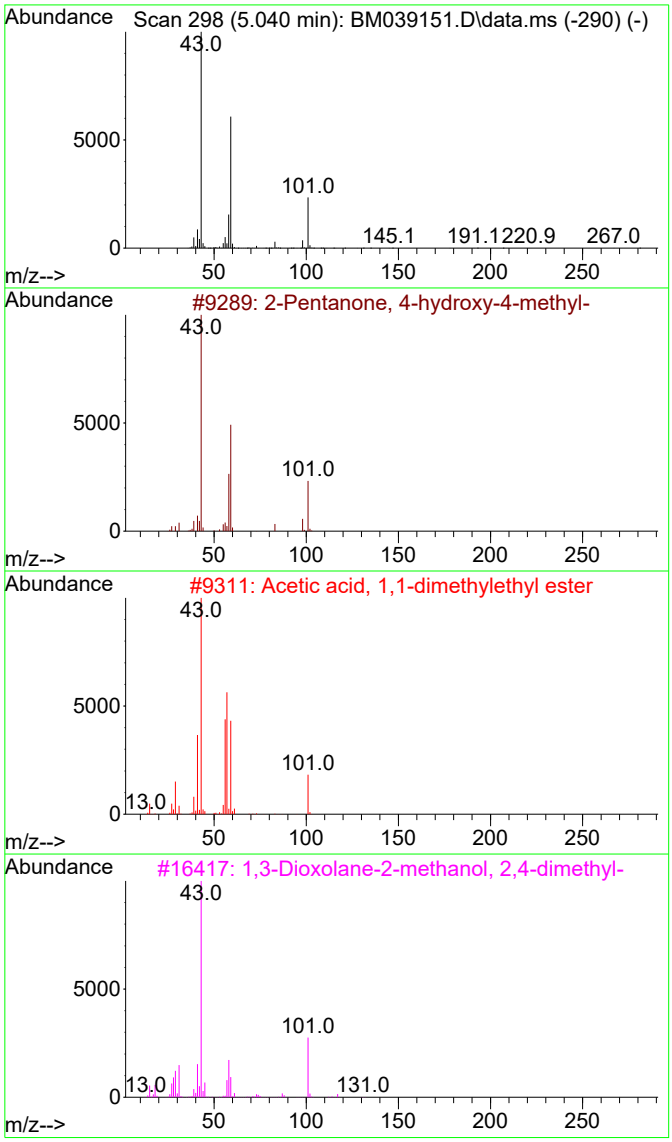
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

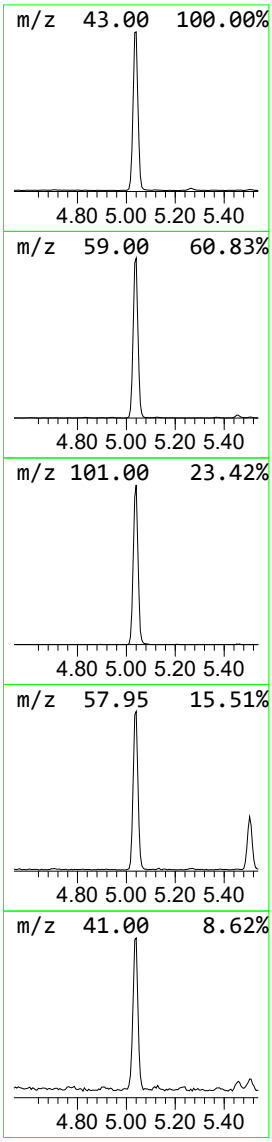
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	16.52 ng	1107340	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

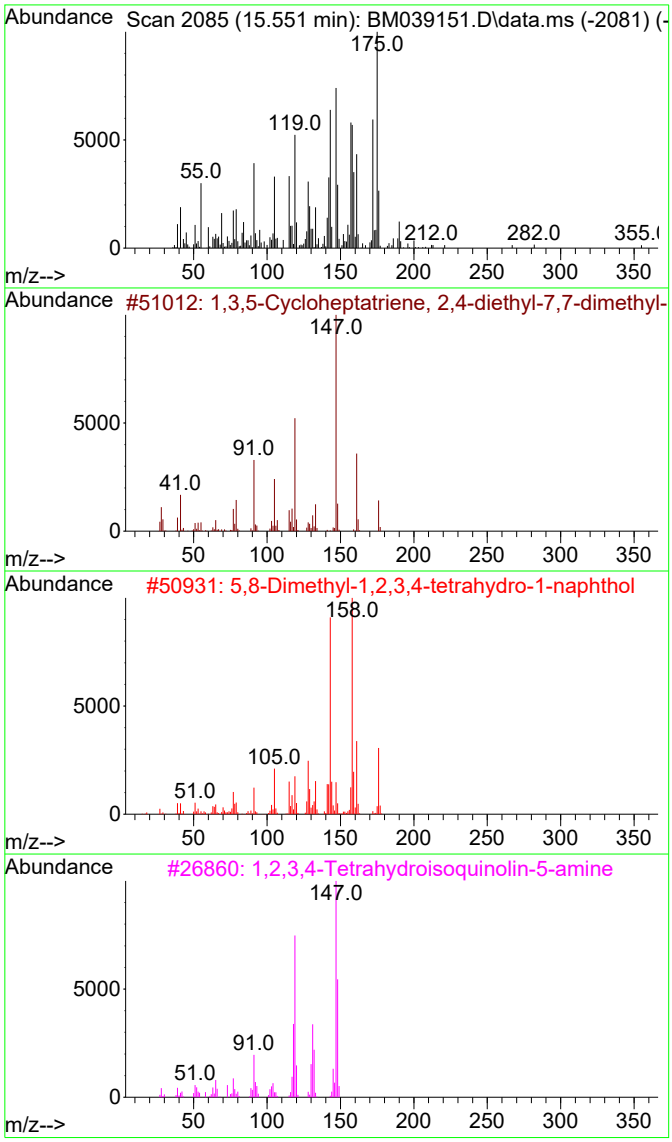
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

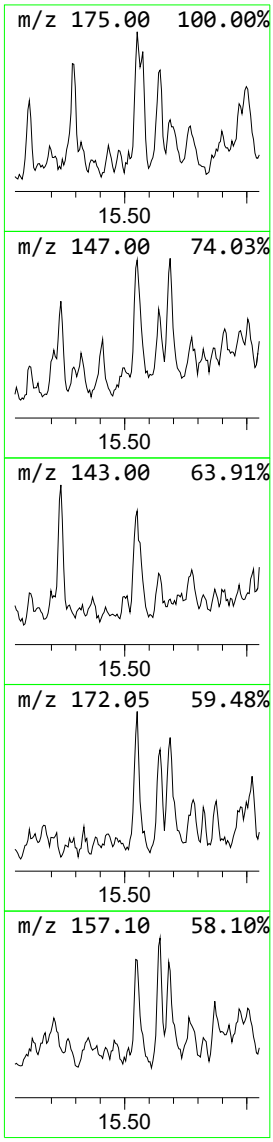
****

Peak Number 2 unknown15.551 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.551	2.96 ng	345763	Acenaphthene-d10	14.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene, 2,4-diet...	176	C13H20	1000156-99-6	30
2	5,8-Dimethyl-1,2,3,4-tetrahydro-...	176	C12H16O	032820-12-5	25
3	1,2,3,4-Tetrahydroisoquinolin-5-...	148	C9H12N2	115955-90-3	25
4	1,3,5-Cycloheptatriene, 3,4-diet...	176	C13H20	1000156-99-7	22
5	1-(4-Tolyl)-1-cyclohexene	172	C13H16	001821-23-4	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

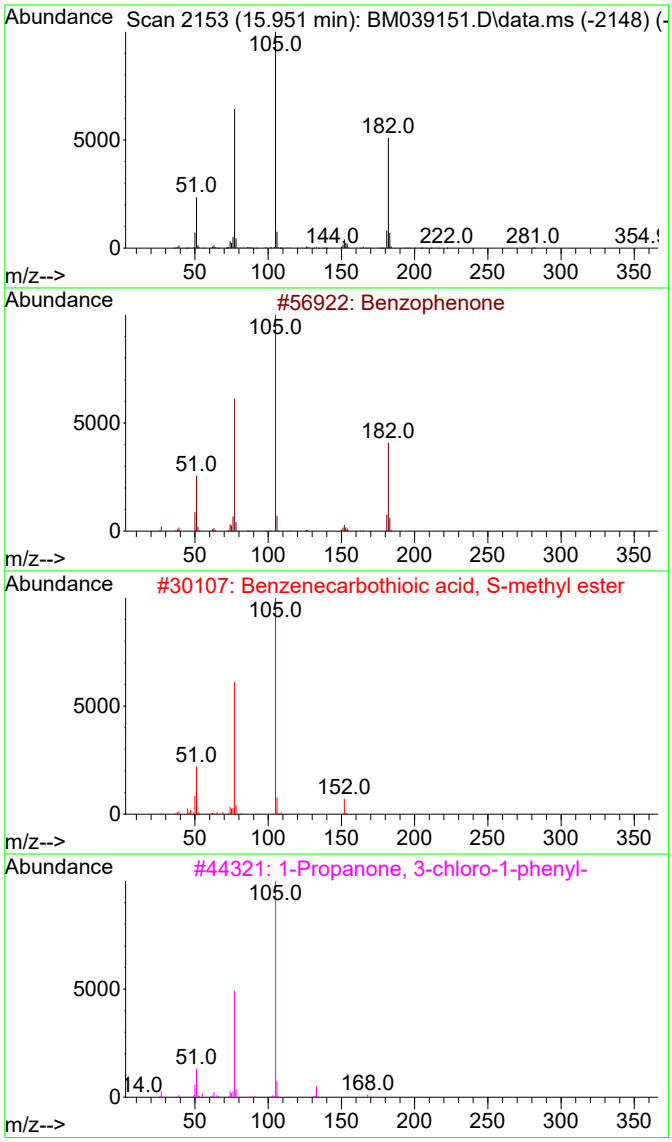
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

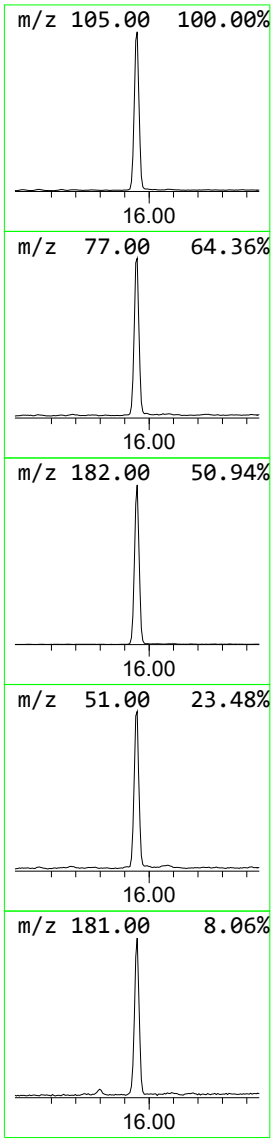
****

Peak Number 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	20.18 ng	2357920	Acenaphthene-d10	14.592

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	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5	Vinyl benzoate	148	C9H8O2	000769-78-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

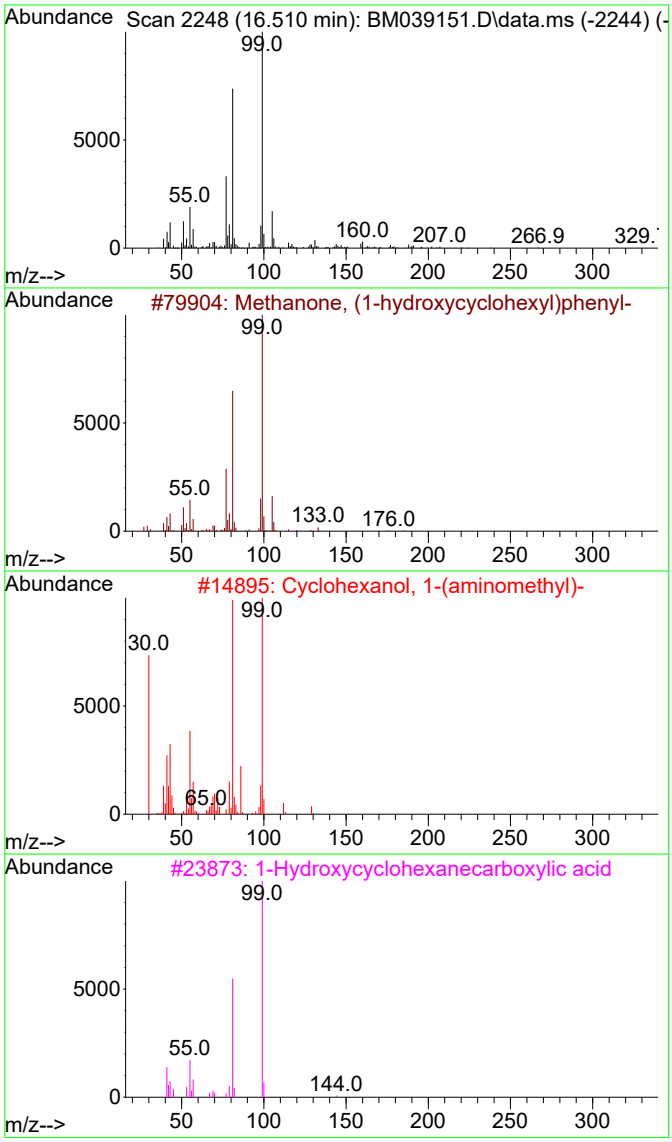
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

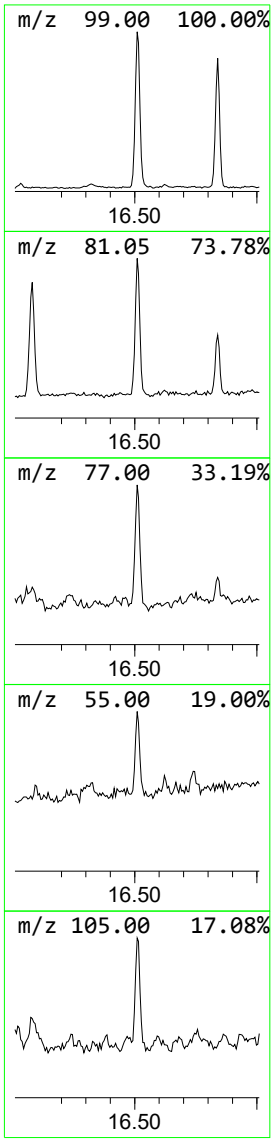
****

Peak Number 4 Methanone, (1-hydroxycycloh... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.510	3.39 ng	405648	Phenanthrene-d10	17.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	86
2	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	64
3	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
4	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	59
5	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

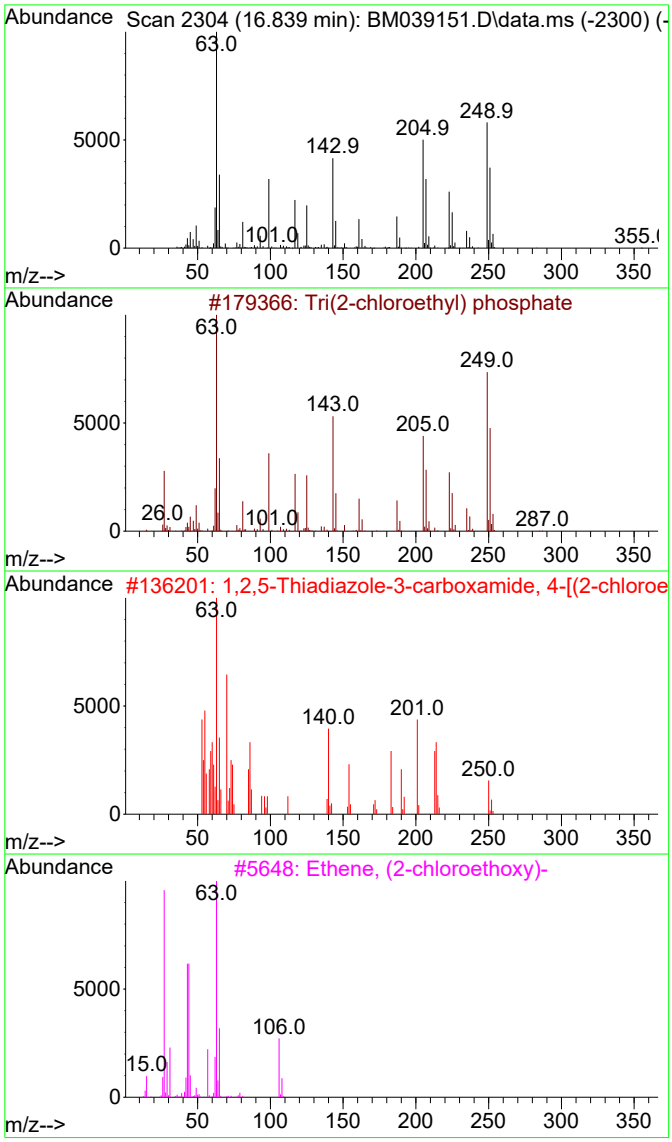
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

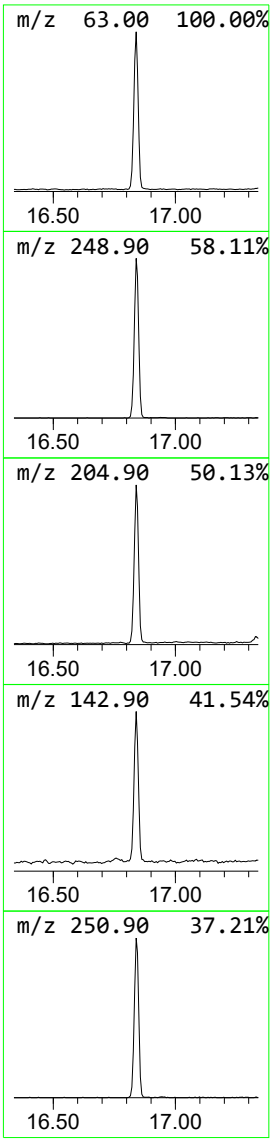
****

Peak Number 5 Tri(2-chloroethyl) phosphate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.839	12.48 ng	1494810	Phenanthrene-d10	17.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tri(2-chloroethyl) phosphate	284	C6H12Cl3O4P	000115-96-8	95
2	1,2,5-Thiadiazole-3-carboxamide,...	250	C7H11ClN4O2S	147194-45-4	47
3	Ethene, (2-chloroethoxy)-	106	C4H7ClO	000110-75-8	47
4	1-Chloroethyl sulfone	190	C4H8Cl2O2S	010038-07-0	47
5	Carbonochloridic acid, 2-chloroe...	142	C3H4Cl2O2	000627-11-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

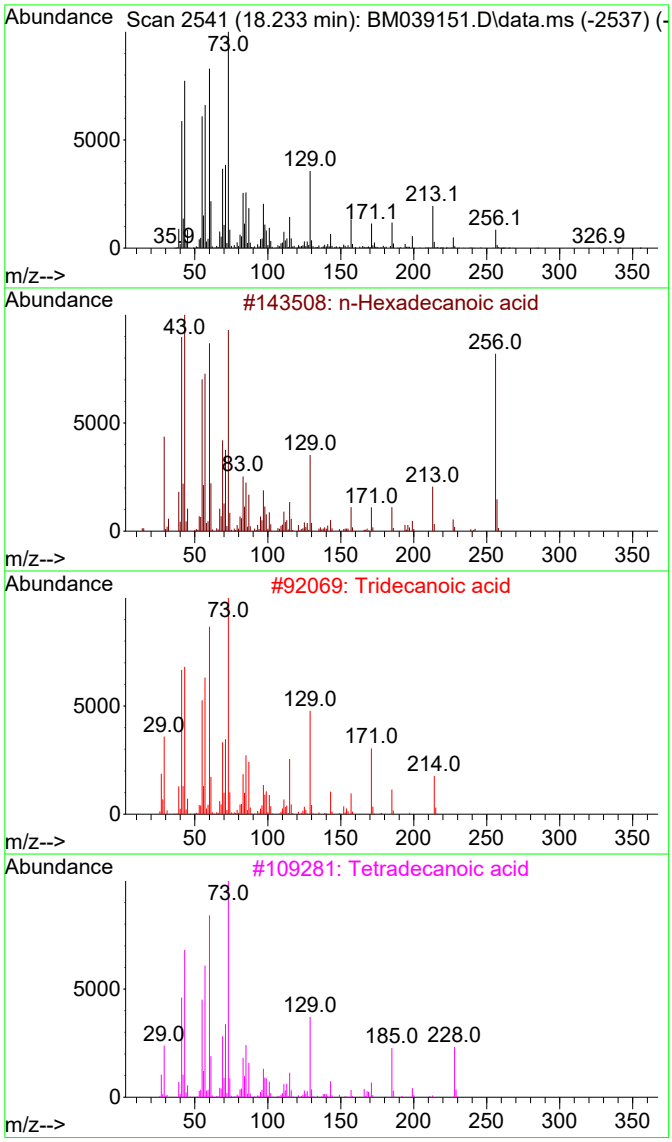
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

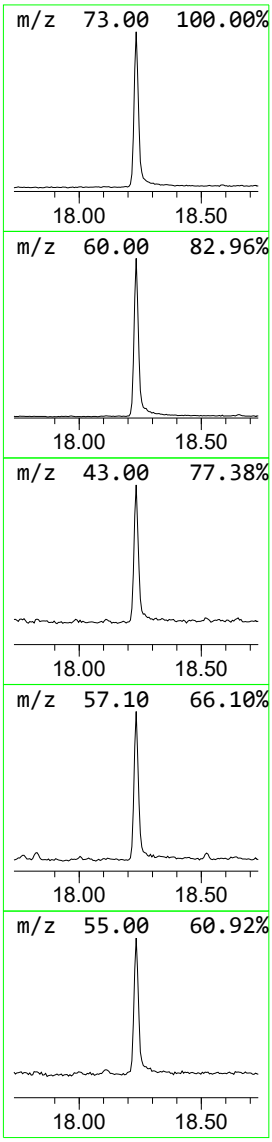
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	14.48 ng	1733830	Phenanthrene-d10	17.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

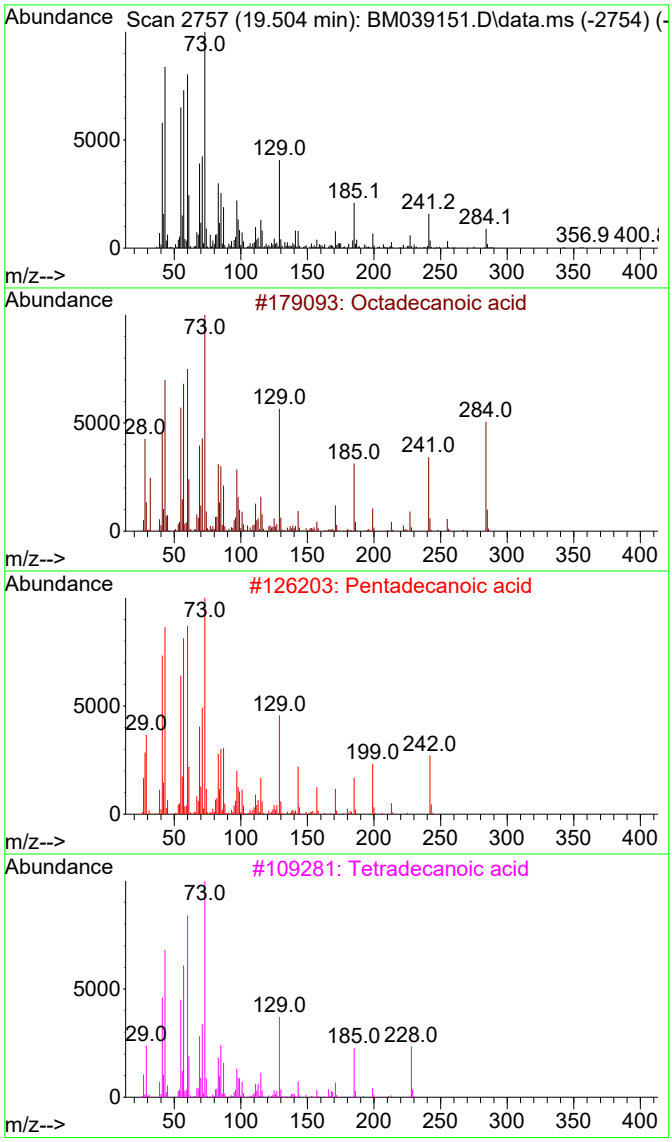
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

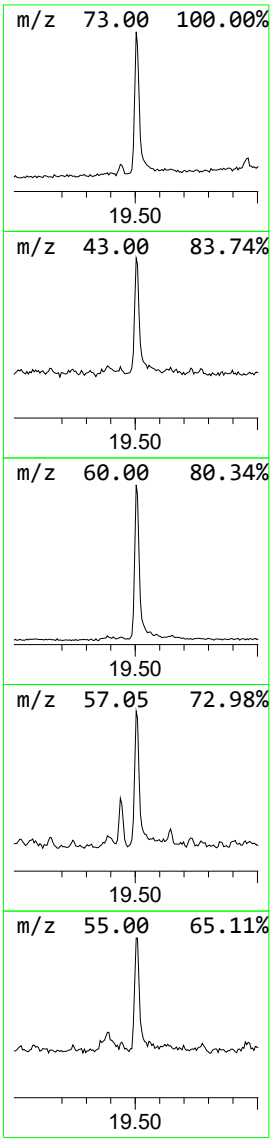
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.504	5.96 ng	788313	Chrysene-d12	21.515

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Tridecane	184	C13H28	000629-50-5	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

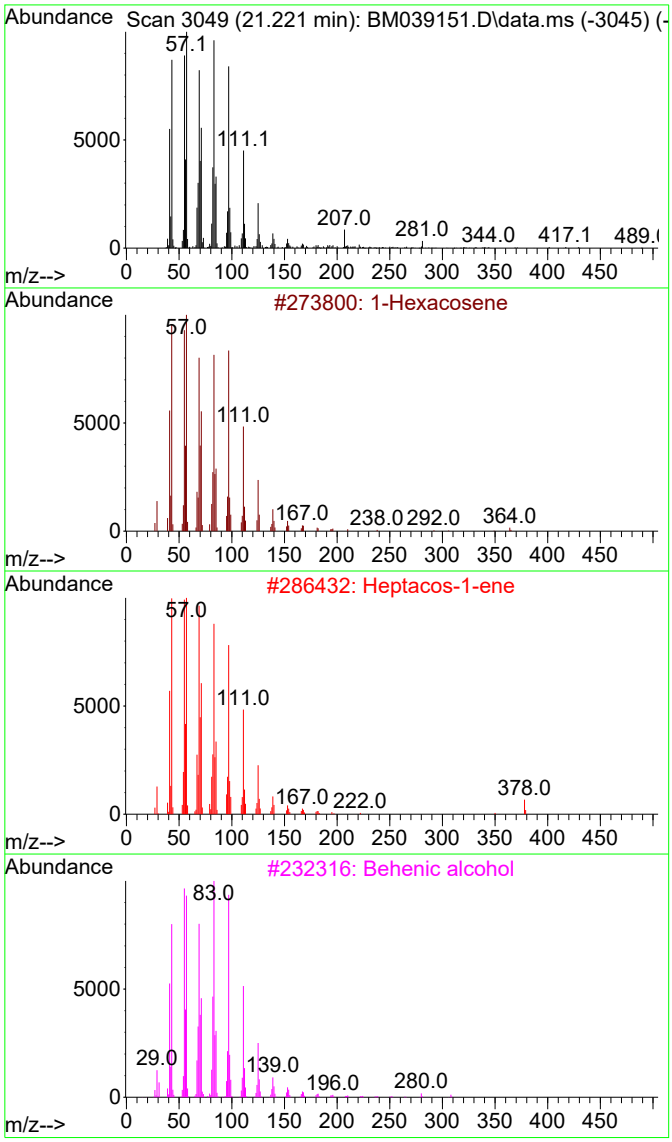
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

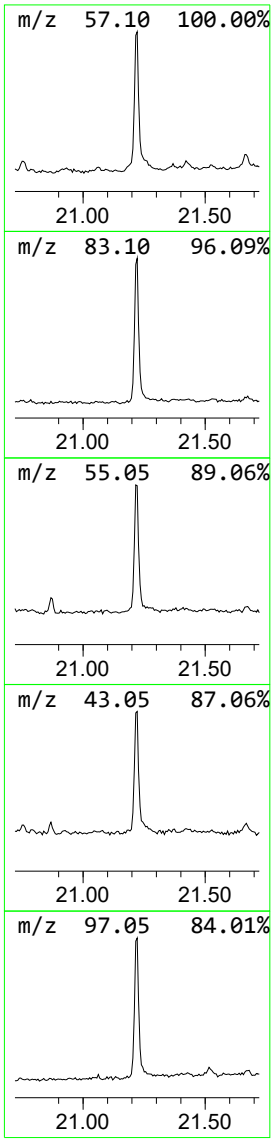
****

Peak Number 8 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	6.53 ng	864461	Chrysene-d12	21.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	Heptacos-1-ene	378	C27H54	015306-27-1	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039151.D
Acq On : 24 Mar 2023 20:59
Operator : CG/JU
Sample : 02069-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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-...	5.040	16.5	ng	1107340	1	7.946	1340350	20.0
unknown15.551	15.551	3.0	ng	345763	3	14.592	2336580	20.0
Benzophenone	15.951	20.2	ng	2357920	3	14.592	2336580	20.0
Methanone, (1-h...	16.510	3.4	ng	405648	4	17.339	2394880	20.0
Tri(2-chloroeth...	16.839	12.5	ng	1494810	4	17.339	2394880	20.0
n-Hexadecanoic ...	18.233	14.5	ng	1733830	4	17.339	2394880	20.0
Octadecanoic acid	19.504	6.0	ng	788313	5	21.515	2647290	20.0
1-Hexacosene	21.221	6.5	ng	864461	5	21.515	2647290	20.0