LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
Data File : BP014121.D
Acq On : 17 Mar 2023 15:15
Operator : CG/JU
Sample : 01928-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
031423-1

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_P\Methods\8270E-BP030623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP014121.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.134	324	331	342	rBV	629942	910515	18.39%	2.983%
2	5.605	405	411	427	rVB	1553071	2333997	47.15%	7.646%
3	7.222	679	686	699	rBV	1492732	2387669	48.23%	7.822%
4	8.063	821	829	836	rBV	453575	713137	14.41%	2.336%
5	9.234	1021	1028	1041	rBV	866339	1479053	29.88%	4.846%
6	10.887	1301	1309	1318	rBV	571364	943283	19.05%	3.090%
7	13.328	1717	1724	1733	rBV	2120190	2980519	60.21%	9.765%
8	14.710	1952	1959	1966	rBV	838345	1233697	24.92%	4.042%
9	16.063	2184	2189	2198	rVB	266312	369236	7.46%	1.210%
10	16.198	2206	2212	2221	rBV	2040770	2886224	58.30%	9.456%
11	16.845	2318	2322	2328	rBV6	34231	61241	1.24%	0.201%
12	17.463	2421	2427	2432	rBV	1108069	1582682	31.97%	5.185%
13	18.204	2549	2553	2558	rBV6	37220	75029	1.52%	0.246%
14	18.328	2569	2574	2598	rBV	872199	1571259	31.74%	5.148%
15	19.457	2761	2766	2774	rVB3	120497	276667	5.59%	0.906%
16	19.551	2778	2782	2796	rBV2	353486	623030	12.59%	2.041%
17	20.004	2854	2859	2864	rBV	4260470	4950364	100.00%	16.218%
18	21.221	3062	3066	3071	rBV	438417	535933	10.83%	1.756%
19	21.551	3117	3122	3127	rBV	1533244	2081522	42.05%	6.819%
20	21.669	3139	3142	3148	rBV2	225535	296343	5.99%	0.971%
21	24.092	3547	3554	3561	rVB2	1055587	2232358	45.09%	7.314%

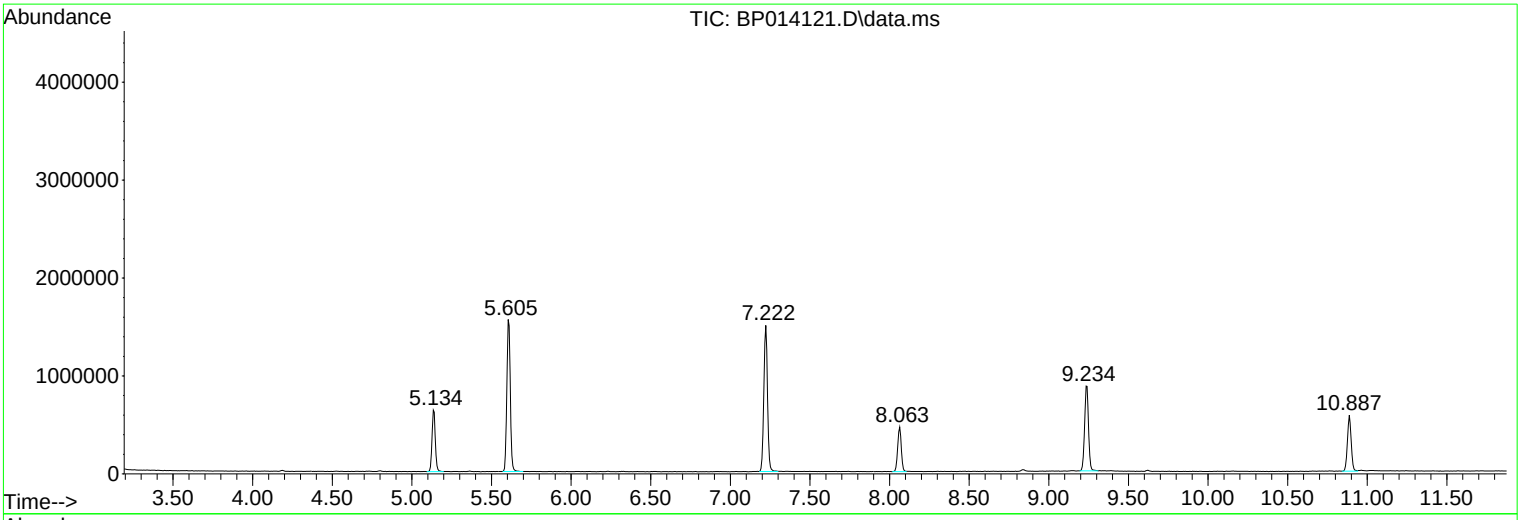
Sum of corrected areas: 30523758

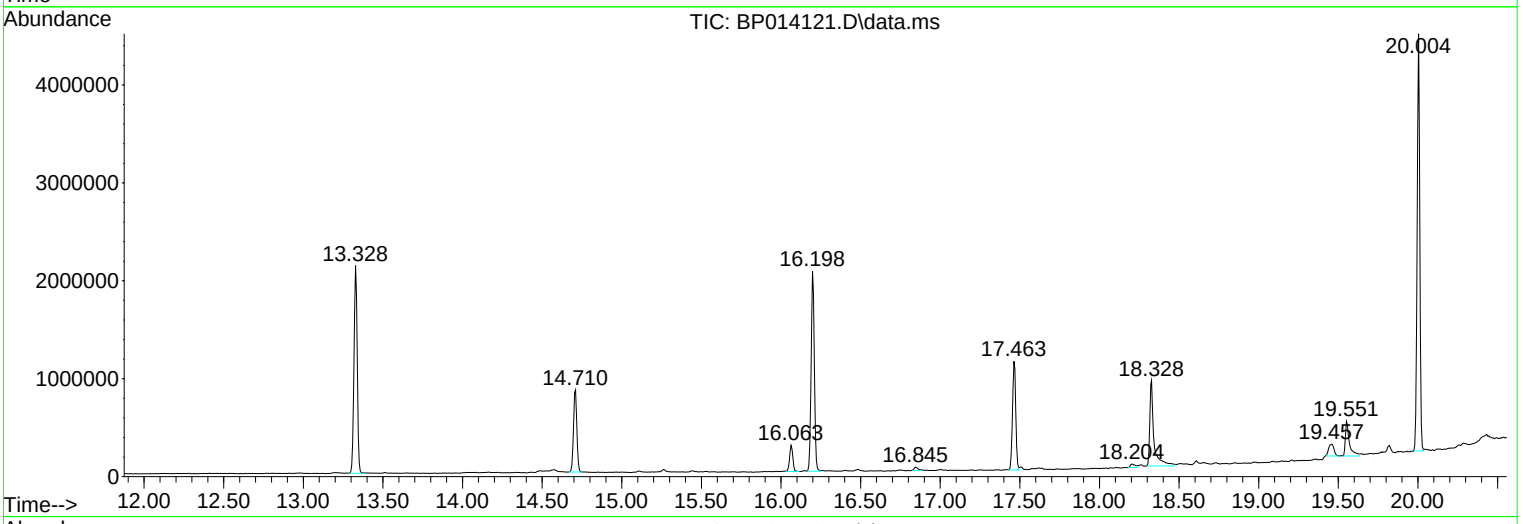
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
Data File : BP014121.D
Acq On : 17 Mar 2023 15:15
Operator : CG/JU
Sample : 01928-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

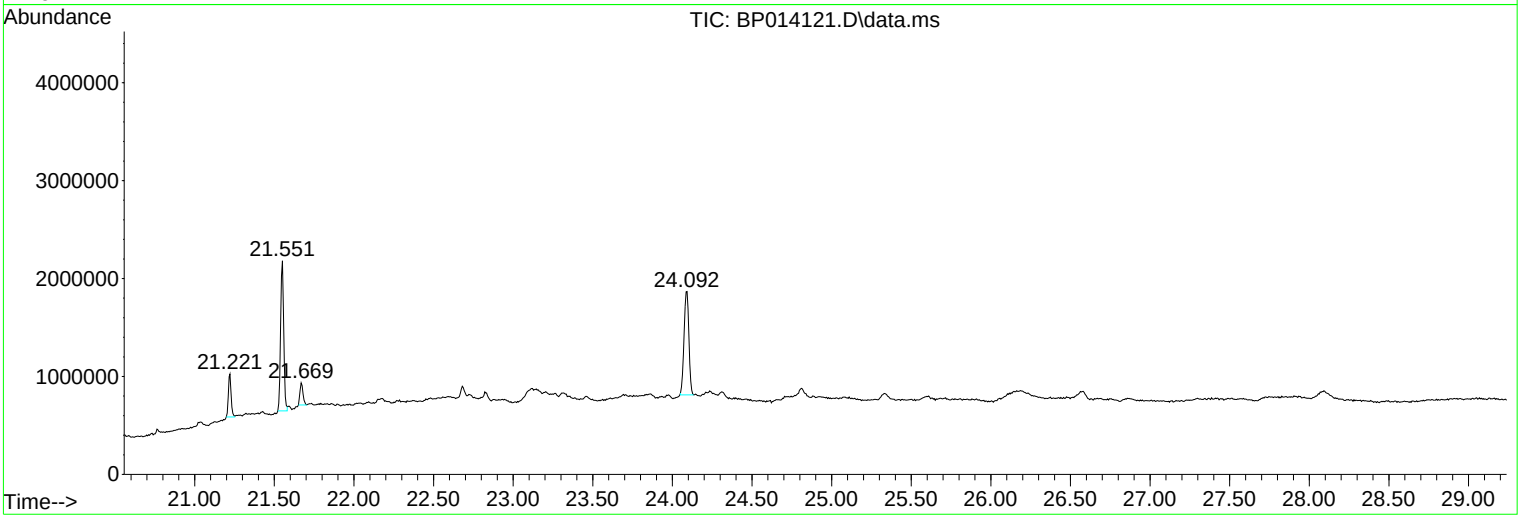
Instrument :
BNA_P
ClientSampleId :
031423-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.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_P\Data\BP031723\
Data File : BP014121.D
Acq On : 17 Mar 2023 15:15
Operator : CG/JU
Sample : 01928-01
Misc :
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Instrument :
BNA_P
ClientSampleId :
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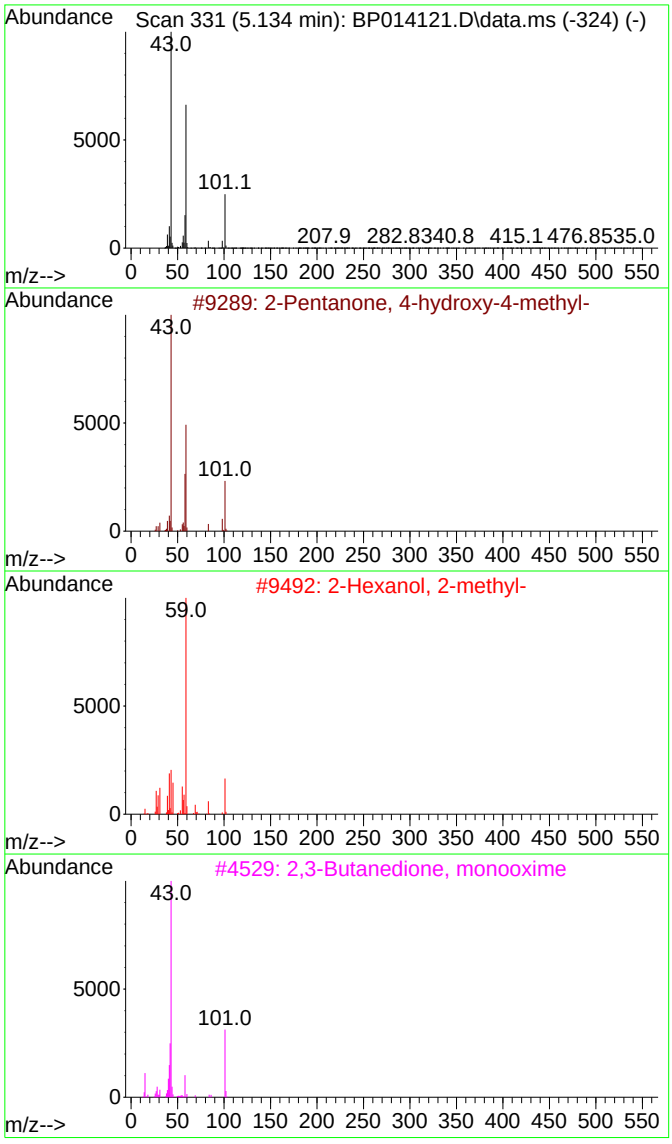
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

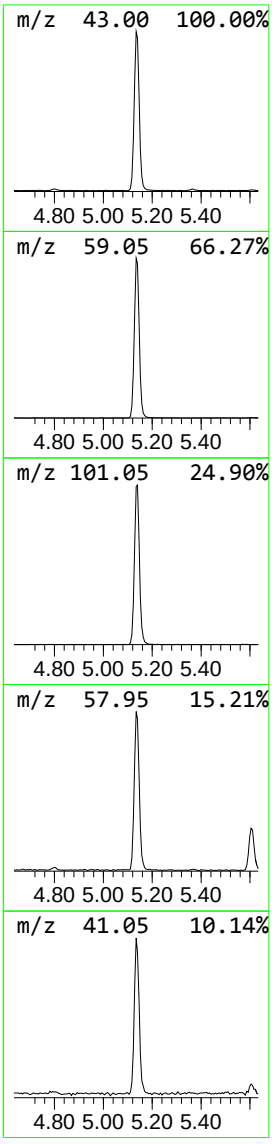
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	25.54 ng	910515	1,4-Dichlorobenzene-d4	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Data File : BP014121.D
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.M
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TIC Library : C:\Database\NIST20.L
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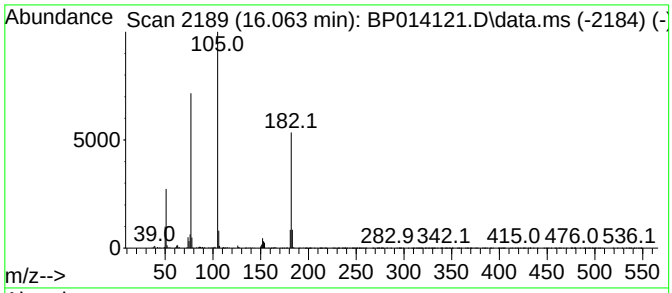
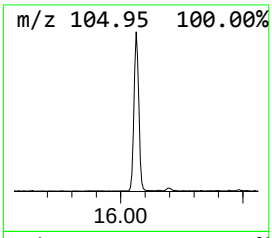
****

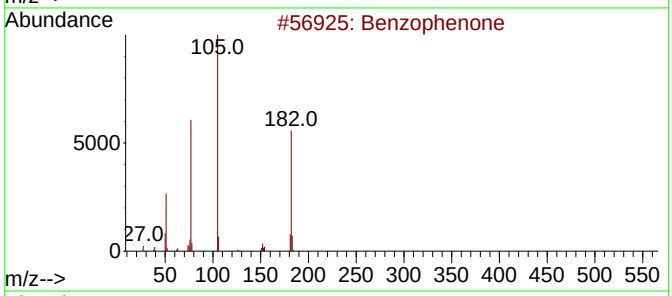
Peak Number 2 Benzophenone Concentration Rank 4

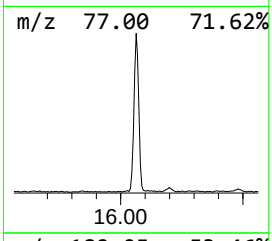
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.063	5.99 ng	369236	Acenaphthene-d10	14.710

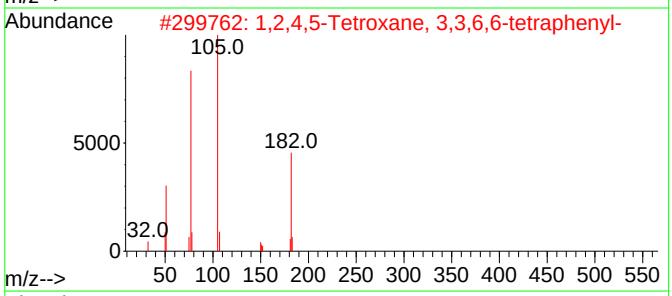
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	64
3	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	64
4	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	45
5	Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	45

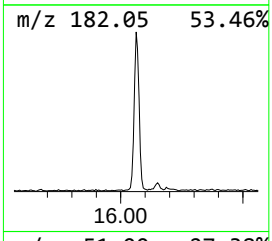


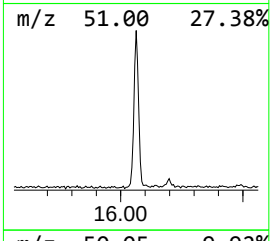


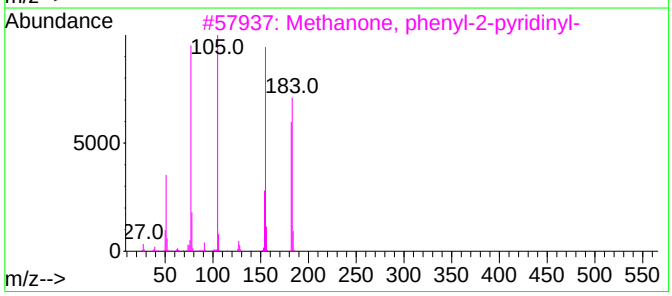


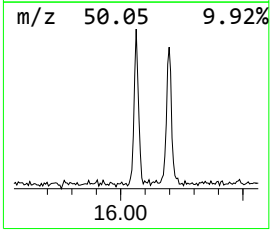












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Data File : BP014121.D
Acq On : 17 Mar 2023 15:15
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Sample : 01928-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
031423-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

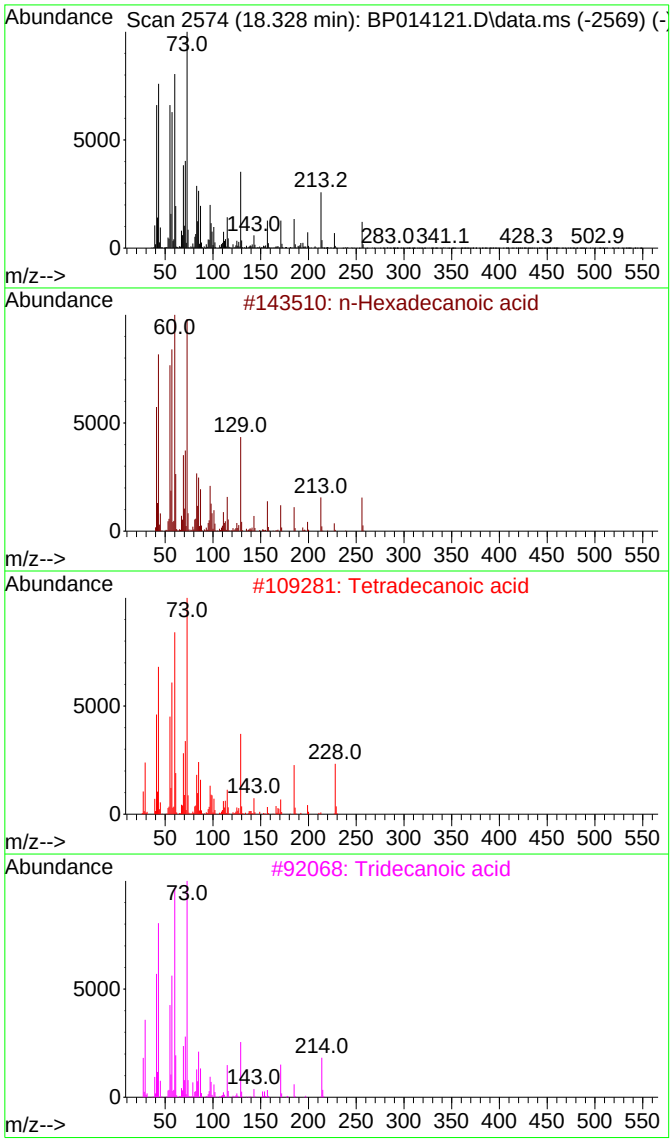
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

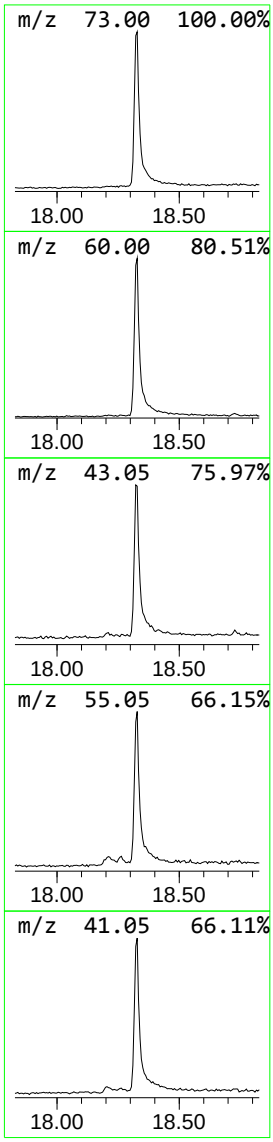
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.328	19.86 ng	1571260	Phenanthrene-d10	17.463

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	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





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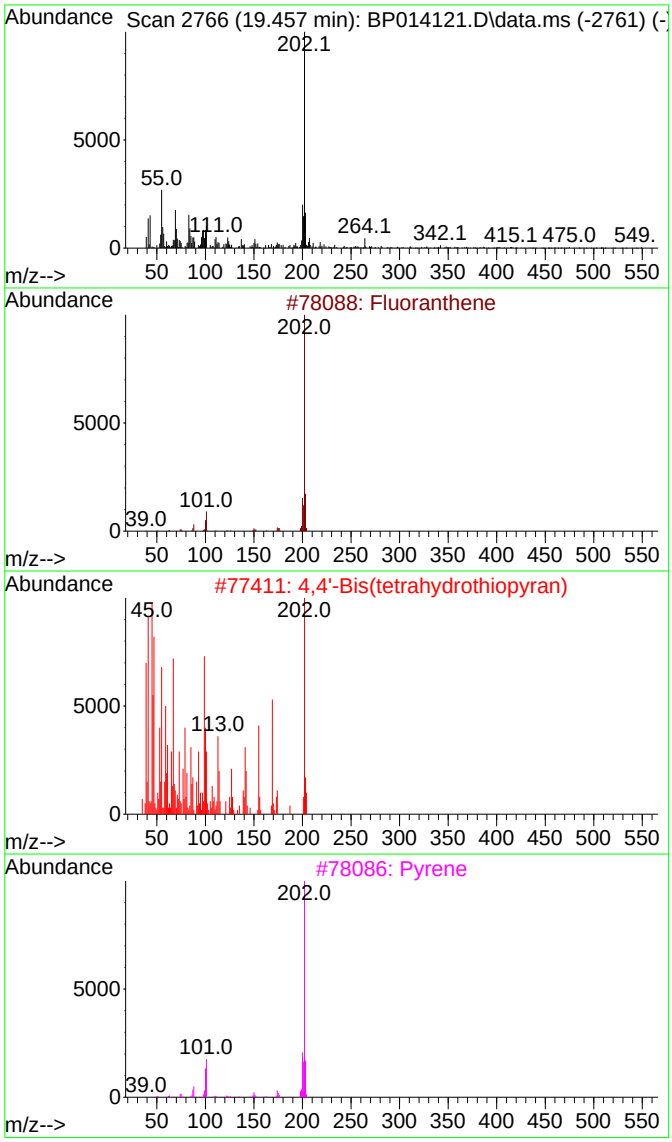
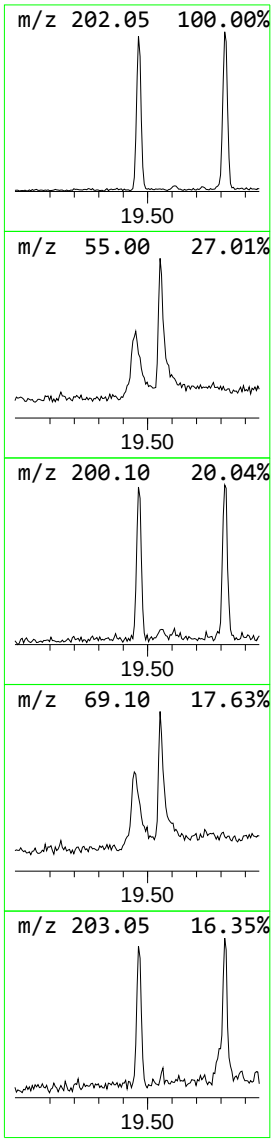
****

Peak Number 4 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.457	3.50 ng	276667	Phenanthrene-d10	17.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	92
2	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	91
3	Pyrene	202	C16H10	000129-00-0	70
4	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
5	Fellutanine A, 4TMS	660	C34H52N4O2Si4	1000503-33-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
Data File : BP014121.D
Acq On : 17 Mar 2023 15:15
Operator : CG/JU
Sample : 01928-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
031423-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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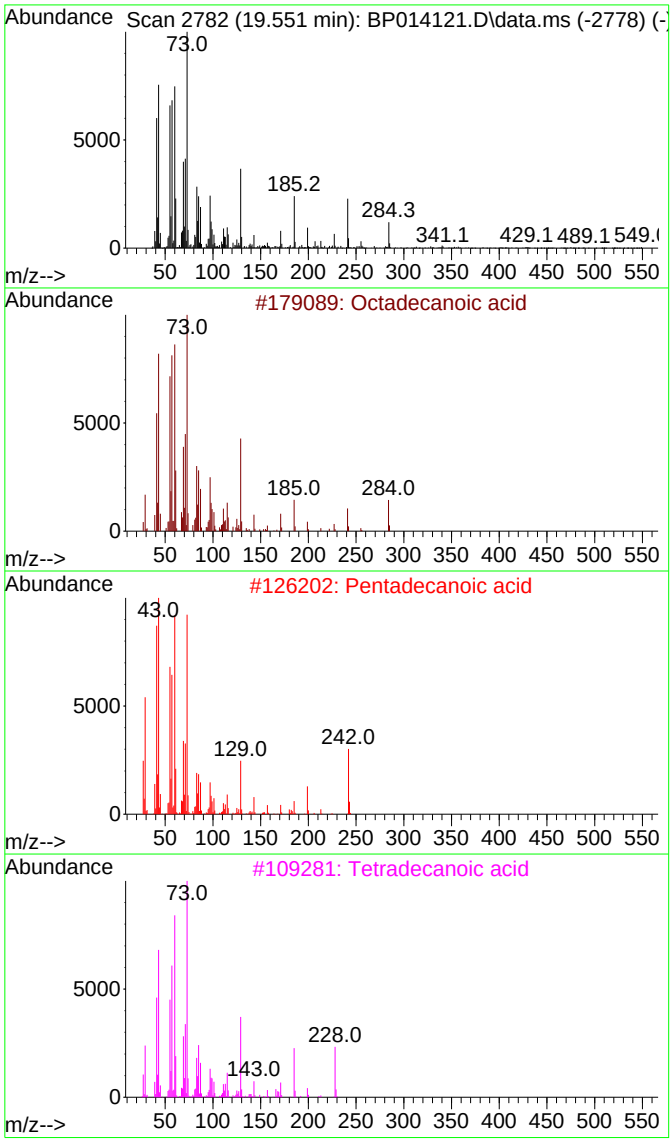
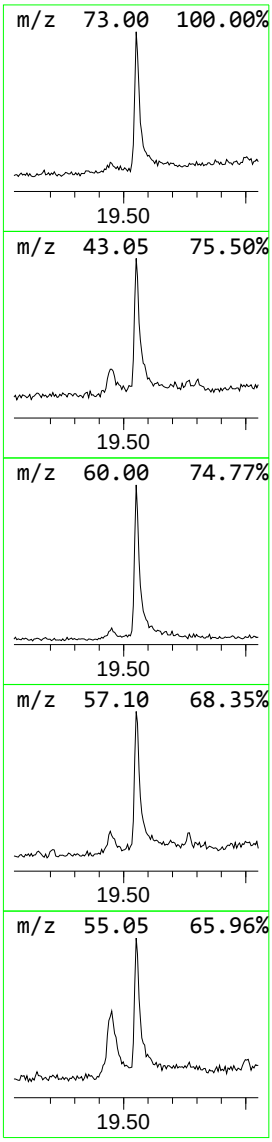
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	5.99 ng	623030	Chrysene-d12	21.551

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Docosanoic acid	340	C22H44O2	000112-85-6	80
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80





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Operator : CG/JU
Sample : 01928-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
031423-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

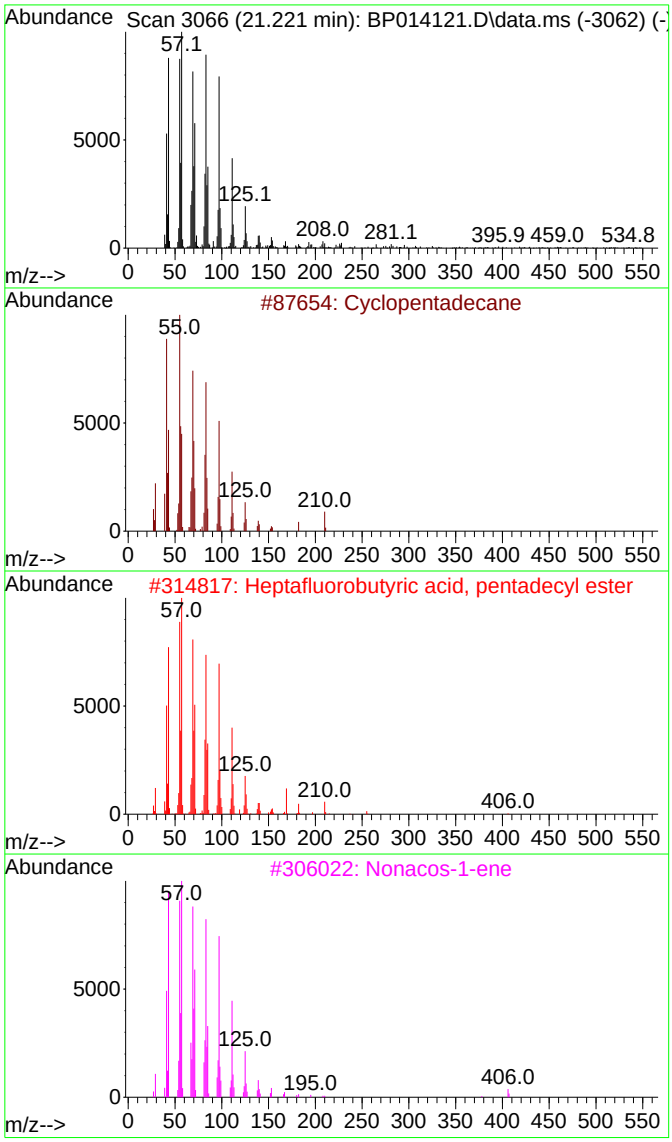
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

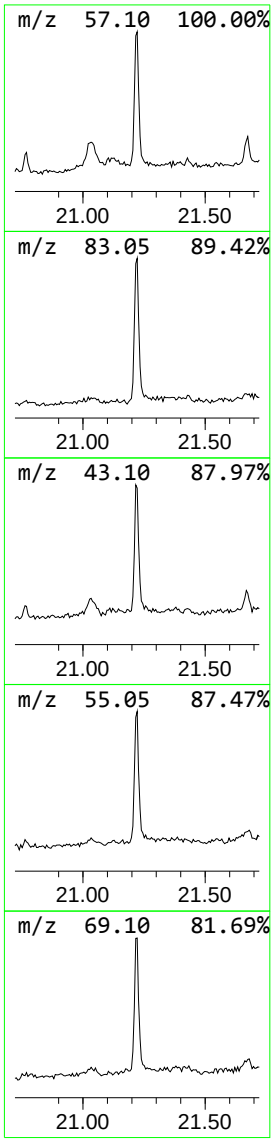
****

Peak Number 6 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	5.15 ng	535933	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Nonacos-1-ene	406	C29H58	018835-35-3	94
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

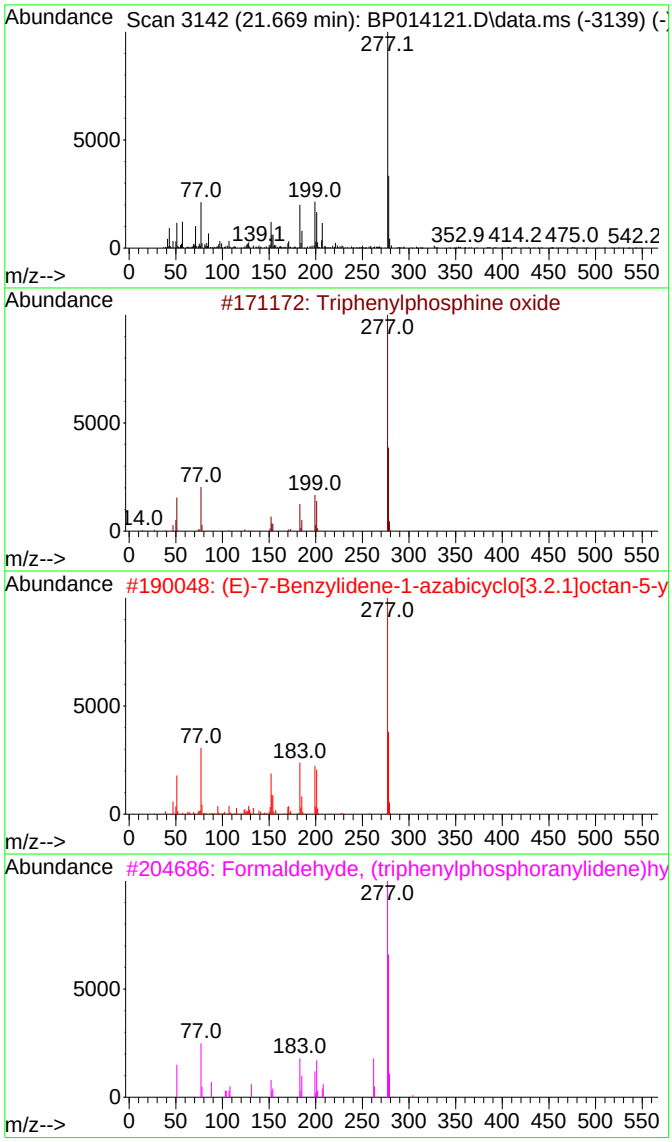
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

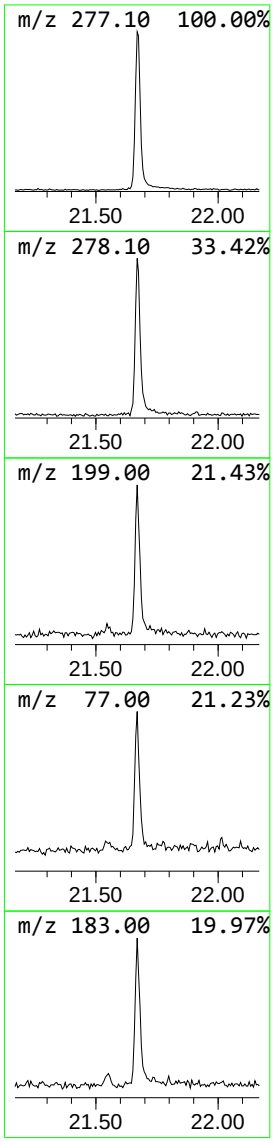
****

Peak Number 7 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.669	2.85 ng	296343	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	83
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	53
4	Dimethoxymethyl-hydroxy-tripheny...	354	C21H23O3P	1000132-00-1	47
5	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
Data File : BP014121.D
Acq On : 17 Mar 2023 15:15
Operator : CG/JU
Sample : 01928-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
031423-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.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-...	5.134	25.5	ng	910515	1	8.063	713137	20.0
Benzophenone	16.063	6.0	ng	369236	3	14.710	1233700	20.0
n-Hexadecanoic ...	18.328	19.9	ng	1571260	4	17.463	1582680	20.0
4,4'-Bis(tetrah...	19.457	3.5	ng	276667	4	17.463	1582680	20.0
Octadecanoic acid	19.551	6.0	ng	623030	5	21.551	2081520	20.0
Cyclopentadecane	21.221	5.2	ng	535933	5	21.551	2081520	20.0
Triphenylphosph...	21.669	2.9	ng	296343	5	21.551	2081520	20.0