LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061825\
Data File : BP024998.D
Acq On : 18 Jun 2025 17:30
Operator : RC/JU
Sample : Q2333-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-13

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-BP060625.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024998.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.967	3	5	22	rVB2	745845	1417014	7.82%	1.819%
2	4.772	307	312	324	rBV	200608	307787	1.70%	0.395%
3	5.237	385	391	414	rVV	2340498	4215736	23.27%	5.413%
4	6.819	654	660	680	rBV	1178547	2617713	14.45%	3.361%
5	7.607	787	794	802	rBV	995954	1583172	8.74%	2.033%
6	8.760	982	990	1012	rBV	2906685	5525992	30.50%	7.095%
7	8.937	1014	1020	1031	rVV	110213	250069	1.38%	0.321%
8	9.784	1155	1164	1173	rBV4	93277	340337	1.88%	0.437%
9	10.378	1258	1265	1286	rBV	1209632	2220732	12.26%	2.851%
10	12.854	1679	1686	1711	rBV	8284906	12573388	69.40%	16.144%
11	14.254	1917	1924	1940	rBV	2022854	2902877	16.02%	3.727%
12	14.401	1942	1949	1966	rBV2	231604	1165287	6.43%	1.496%
13	15.642	2154	2160	2168	rBV	361563	587530	3.24%	0.754%
14	15.783	2176	2184	2203	rBV	6356422	10976171	60.58%	14.093%
15	17.066	2395	2402	2416	rBV2	2316373	3506756	19.36%	4.503%
16	18.001	2556	2561	2570	rBV	305520	586221	3.24%	0.753%
17	19.330	2782	2787	2794	rBV2	185254	365247	2.02%	0.469%
18	19.783	2858	2864	2878	rBV	12798904	18117315	100.00%	23.263%
19	21.154	3094	3097	3107	rVB4	114424	187670	1.04%	0.241%
20	21.495	3149	3155	3168	rBV2	2063593	3917498	21.62%	5.030%
21	21.660	3179	3183	3189	rBV	325600	488537	2.70%	0.627%
22	24.759	3703	3710	3730	rVB	1575386	4028880	22.24%	5.173%

Sum of corrected areas: 77881929

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061825\
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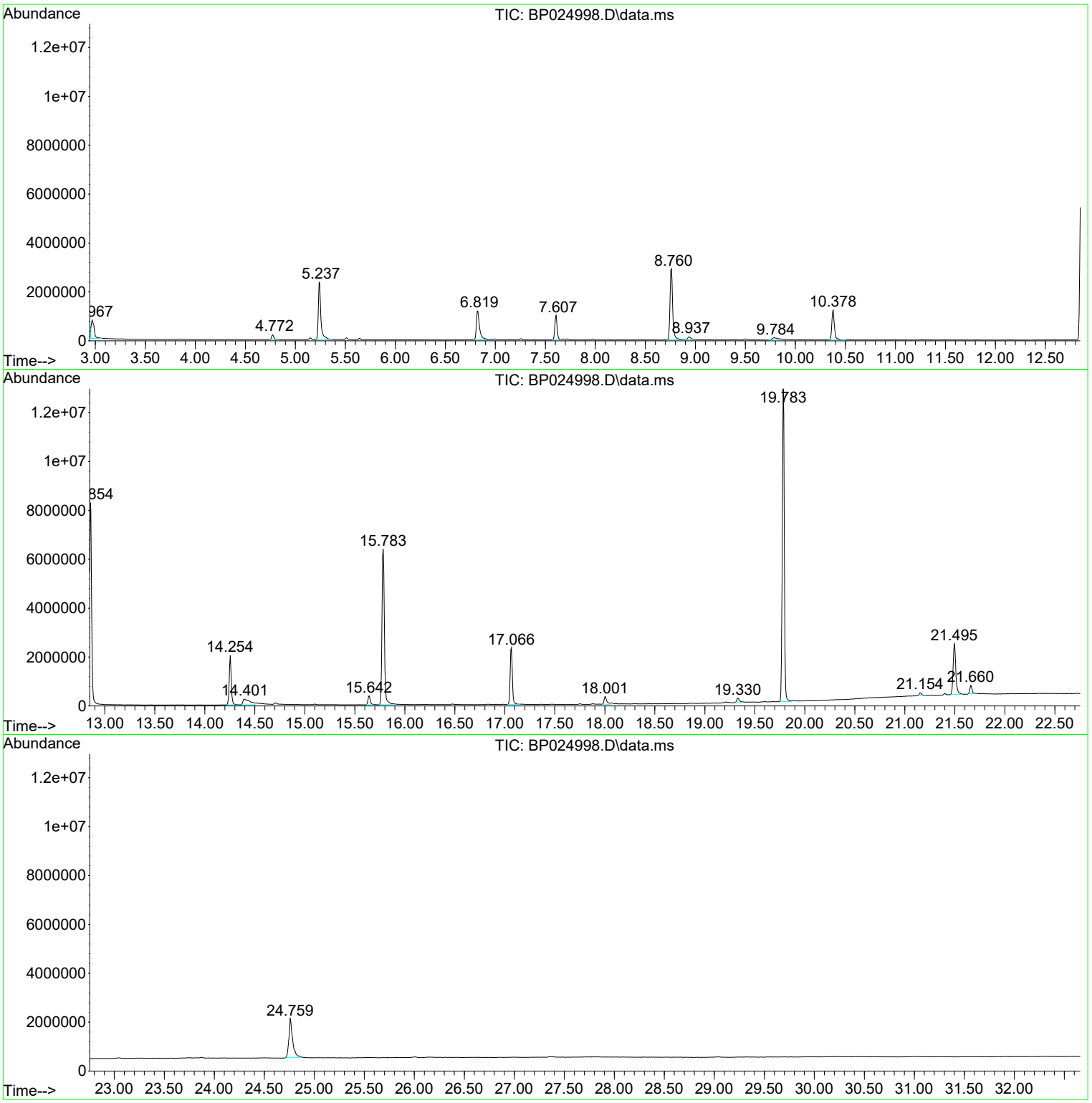
ClientSampleId :
MW-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BP024998.D
Acq On : 18 Jun 2025 17:30
Operator : RC/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

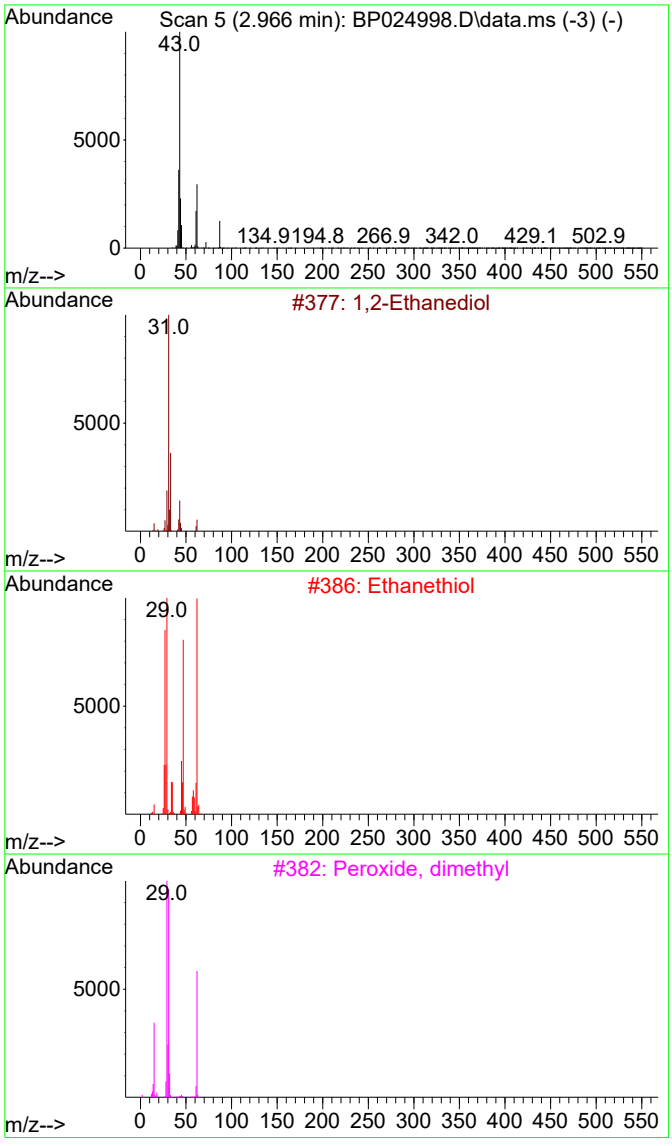
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

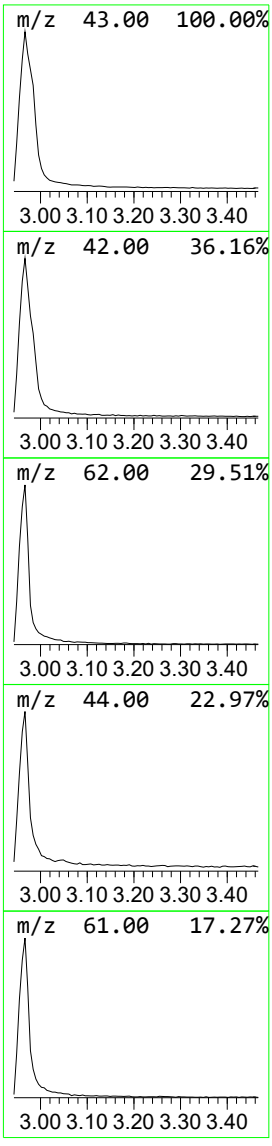
****

Peak Number 1 unknown2.996 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.966	17.90 ng	1417010	1,4-Dichlorobenzene-d4	7.607

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol	62	C2H6O2	000107-21-1	9
2	Ethanethiol	62	C2H6S	000075-08-1	5
3	Peroxide, dimethyl	62	C2H6O2	000690-02-8	4
4	1-Pentanamine	87	C5H13N	000110-58-7	4
5	1,8-Diamino-3,6-dioxaoctane	148	C6H16N2O2	000929-59-9	4





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BNA_P
ClientSampleId :
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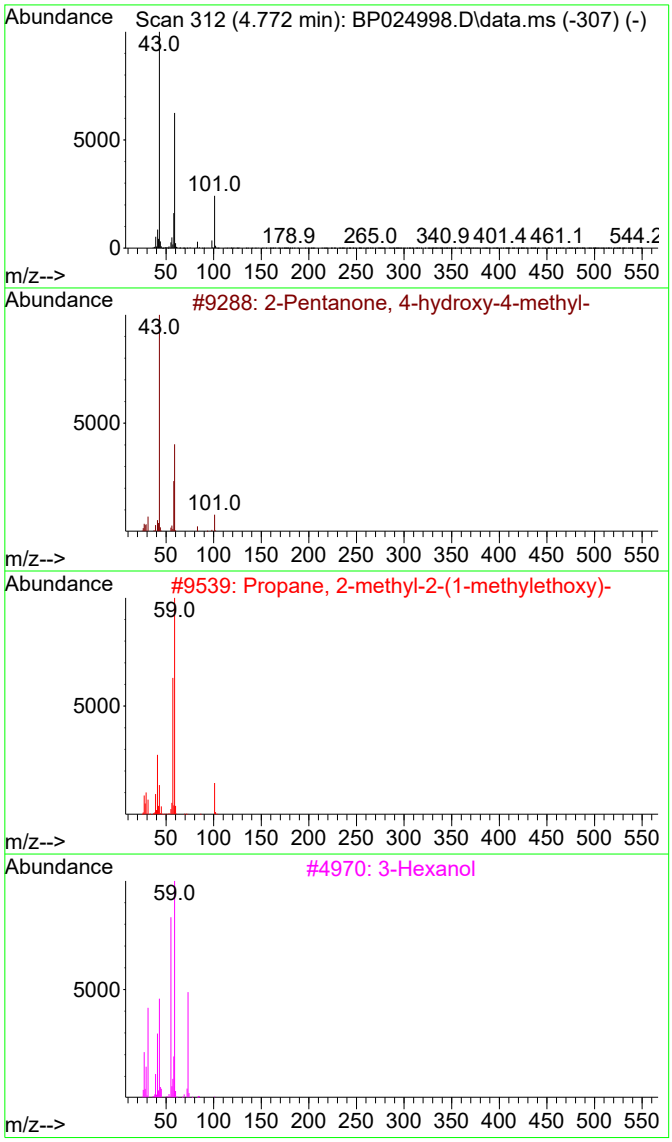
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

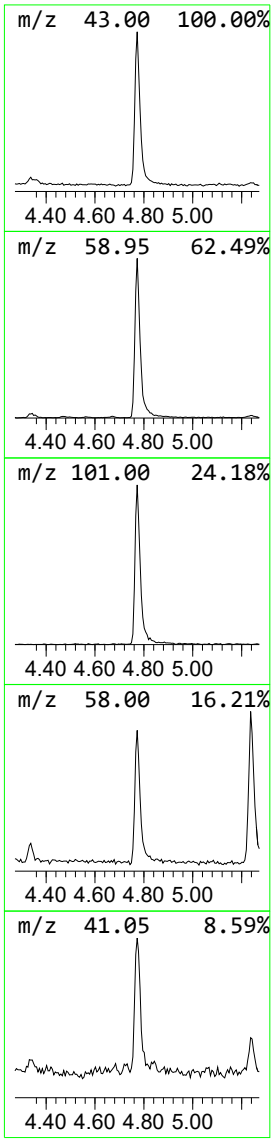
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.772	3.89 ng	307787	1,4-Dichlorobenzene-d4	7.607

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Data File : BP024998.D
Acq On : 18 Jun 2025 17:30
Operator : RC/JU
Sample : Q2333-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-13

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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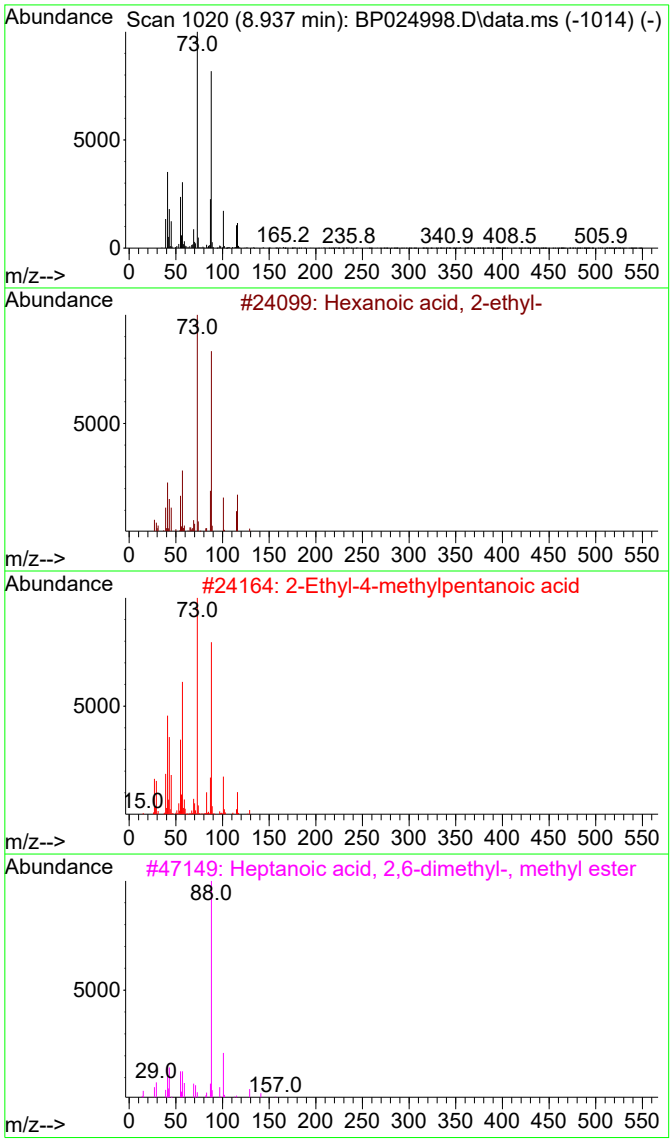
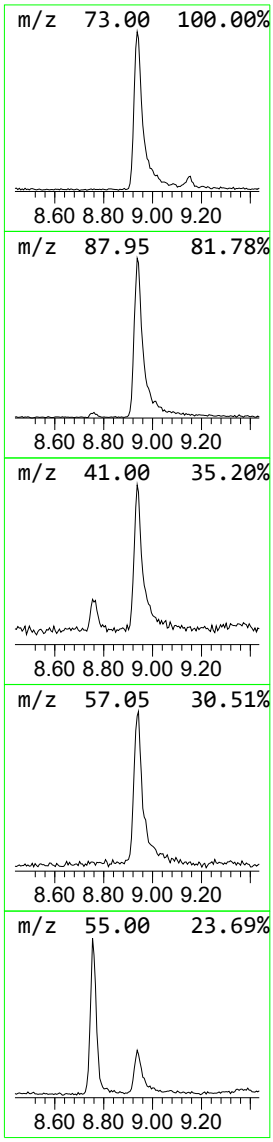
****

Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.937	3.16 ng	250069	1,4-Dichlorobenzene-d4	7.607

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	59
3	Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	47
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40
5	1,4-Dioxane	88	C4H8O2	000123-91-1	37





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Sample : Q2333-05
Misc :
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Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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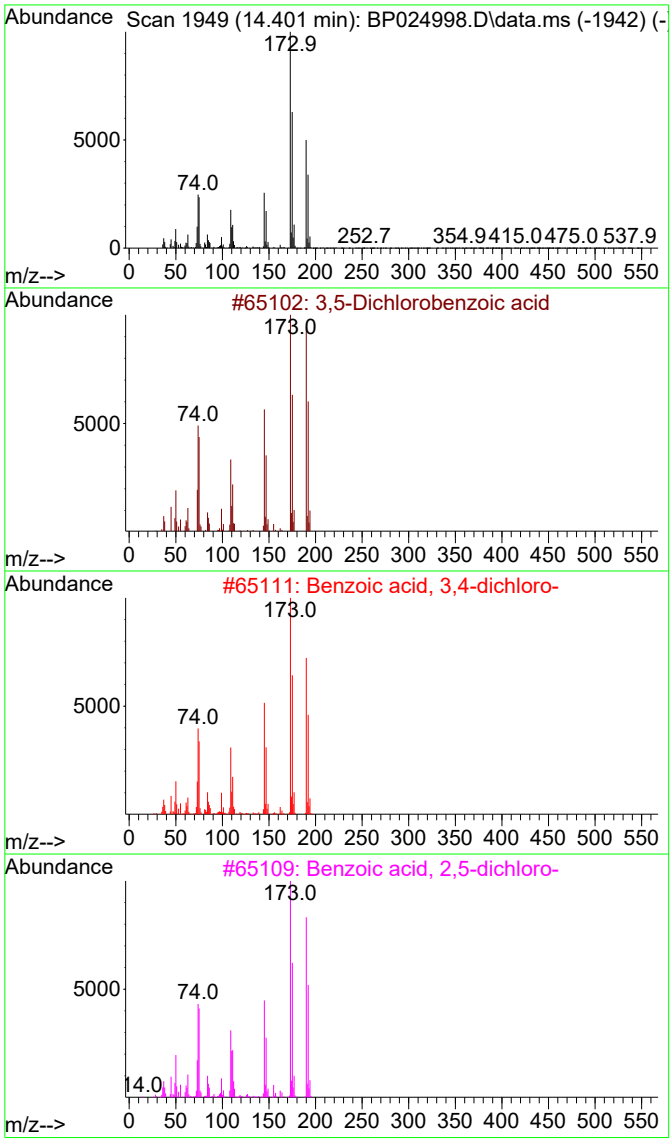
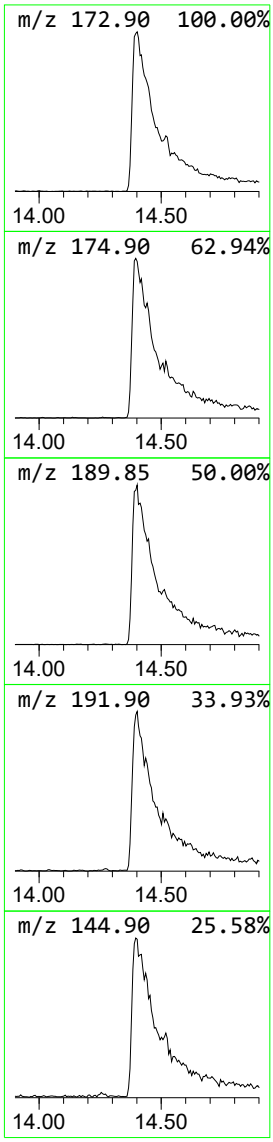
Peak Number 4 3,5-Dichlorobenzoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.401	8.03 ng	1165290	Acenaphthene-d10	14.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	97
2	Benzoic acid, 3,4-dichloro-	190	C7H4Cl2O2	000051-44-5	97
3	Benzoic acid, 2,5-dichloro-	190	C7H4Cl2O2	000050-79-3	97
4	Benzoic acid, 2,6-dichloro-	190	C7H4Cl2O2	000050-30-6	97
5	Benzoic acid, 2,3-dichloro-	190	C7H4Cl2O2	000050-45-3	96





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Instrument :
BNA_P
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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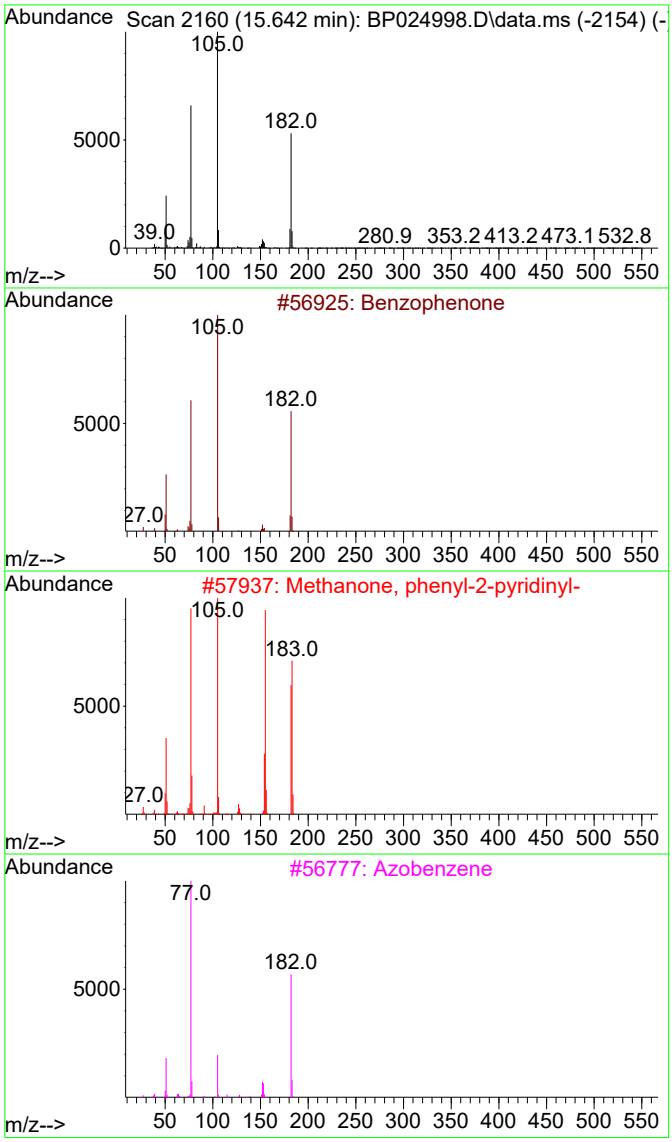
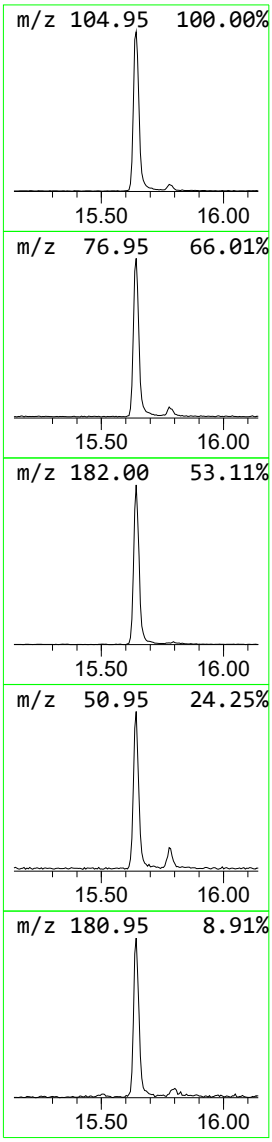
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.642	4.05 ng	587530	Acenaphthene-d10	14.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
3	Azobenzene	182	C12H10N2	000103-33-3	45
4	Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	45
5	1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	27





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

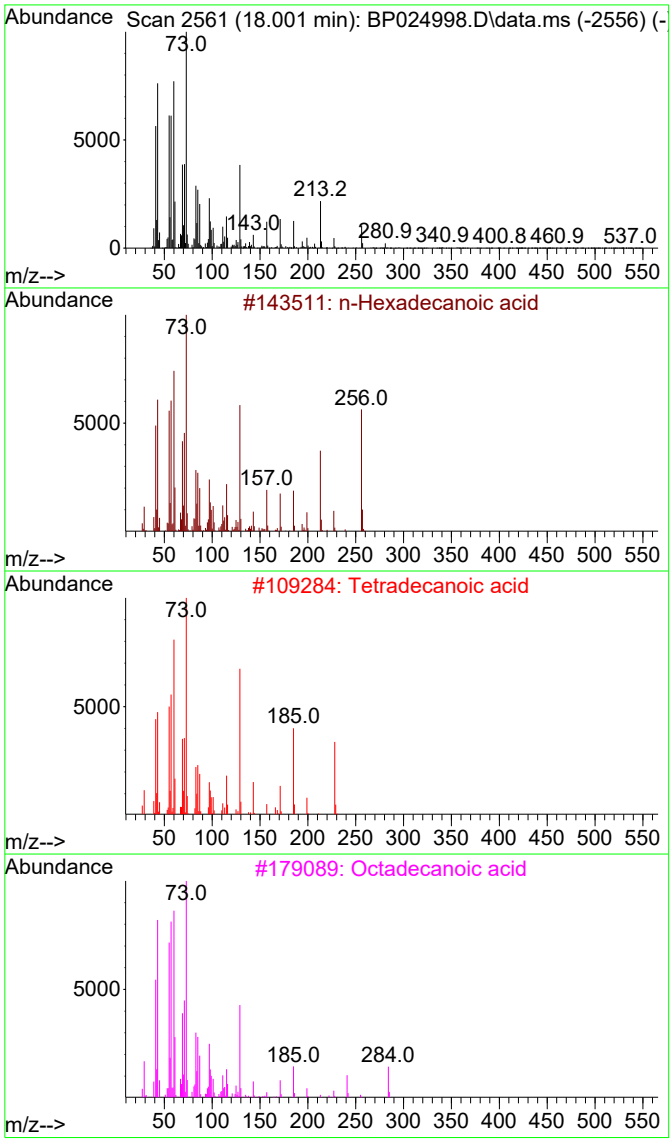
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

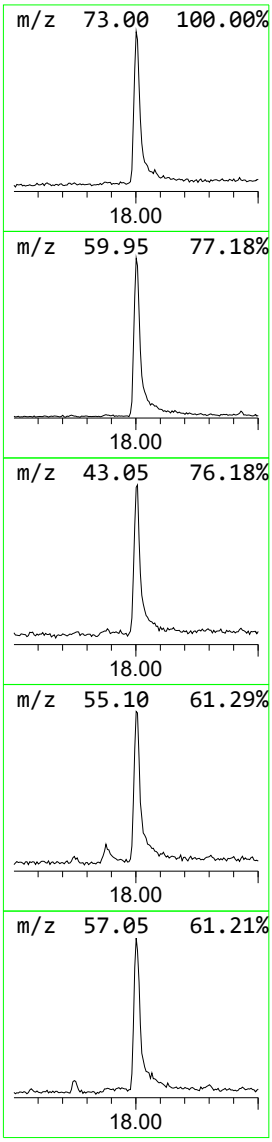
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.001	3.34 ng	586221	Phenanthrene-d10	17.066

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	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	81





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

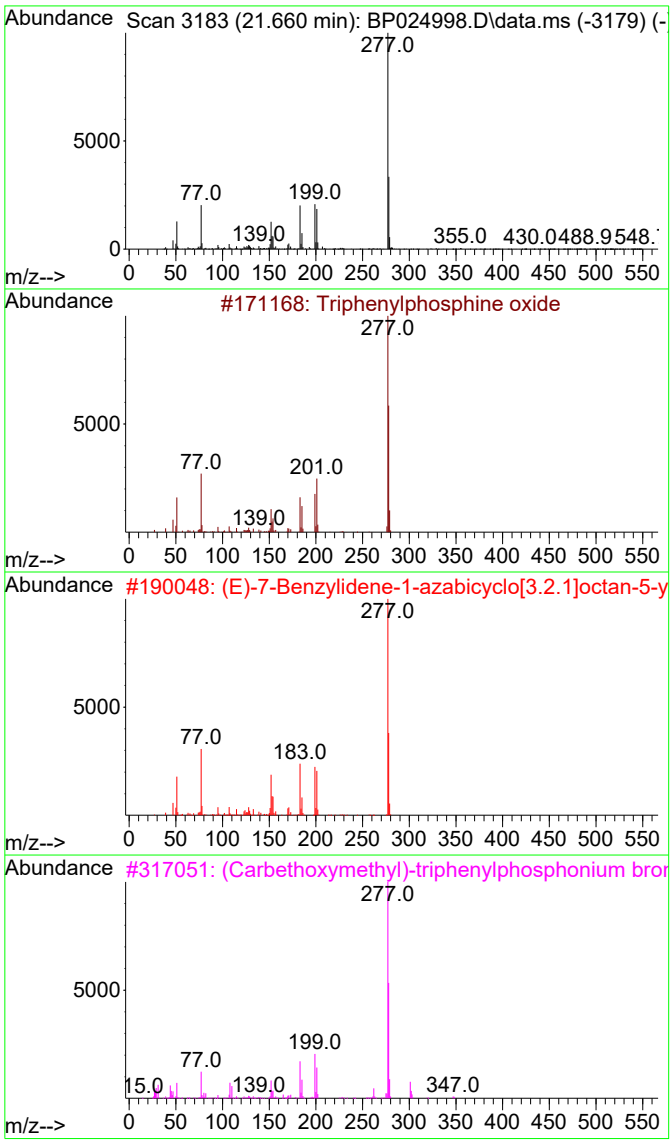
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

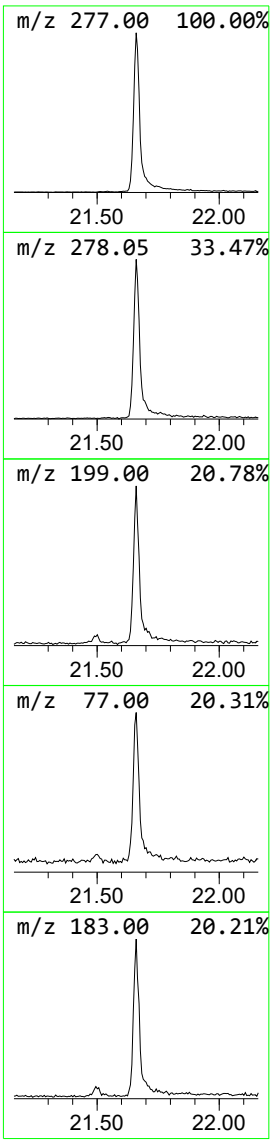
****

Peak Number 7 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.660	2.49 ng	488537	Chrysene-d12	21.495

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	59
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.996	2.966	17.9	ng	1417010	1	7.607	1583170	20.0
2-Pentanone, 4-...	4.772	3.9	ng	307787	1	7.607	1583170	20.0
Hexanoic acid, ...	8.937	3.2	ng	250069	1	7.607	1583170	20.0
3,5-Dichloroben...	14.401	8.0	ng	1165290	3	14.254	2902880	20.0
Benzophenone	15.642	4.0	ng	587530	3	14.254	2902880	20.0
n-Hexadecanoic ...	18.001	3.3	ng	586221	4	17.066	3506760	20.0
Triphenylphosph...	21.660	2.5	ng	488537	5	21.495	3917500	20.0