LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042225\
Data File : BP024378.D
Acq On : 22 Apr 2025 14:41
Operator : RC/JU
Sample : Q1842-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PL-714-COMP-10

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-BP041425.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.881	300	305	317	rBV	654441	914899	7.44%	1.292%
2	5.340	376	383	400	rBV	2926721	4118898	33.49%	5.819%
3	5.940	479	485	492	rVB	106420	153636	1.25%	0.217%
4	6.905	640	649	664	rBV	2864642	4611416	37.50%	6.515%
5	7.716	779	787	794	rBV	664696	1025813	8.34%	1.449%
6	8.863	975	982	993	rBV	1705755	2783870	22.64%	3.933%
7	10.493	1251	1259	1269	rVB	870198	1451759	11.81%	2.051%
8	12.963	1672	1679	1693	rBV	4955532	6940747	56.44%	9.805%
9	14.351	1909	1915	1922	rBV	1483548	2020828	16.43%	2.855%
10	15.745	2146	2152	2155	rBV	616748	807332	6.56%	1.141%
11	15.810	2155	2163	2168	rBV2	274836	617357	5.02%	0.872%
12	15.875	2168	2174	2183	rBV	4438541	7561398	61.49%	10.682%
13	16.557	2283	2290	2301	rBV4	127486	263838	2.15%	0.373%
14	17.157	2385	2392	2397	rBV	1564778	2472599	20.11%	3.493%
15	17.204	2397	2400	2407	rVB	192685	294861	2.40%	0.417%
16	17.581	2458	2464	2474	rVB2	82750	167371	1.36%	0.236%
17	18.104	2546	2553	2560	rBV	4080760	6154813	50.05%	8.695%
18	18.381	2595	2600	2606	rBV	284231	554485	4.51%	0.783%
19	18.433	2606	2609	2622	rVB2	164044	411364	3.35%	0.581%
20	18.545	2624	2628	2632	rVB	138300	159423	1.30%	0.225%
21	19.010	2702	2707	2714	rBV3	129814	223882	1.82%	0.316%
22	19.292	2748	2755	2766	rBV	717007	1228004	9.99%	1.735%
23	19.433	2775	2779	2794	rBV	1541217	2251382	18.31%	3.181%
24	19.669	2815	2819	2823	rVB	635973	726110	5.90%	1.026%
25	19.880	2849	2855	2865	rBV	9658771	12297788	100.00%	17.373%
26	20.198	2905	2909	2910	rBV2	110977	143999	1.17%	0.203%
27	20.739	2997	3001	3007	rVB2	142398	214045	1.74%	0.302%
28	21.280	3088	3093	3107	rVB3	640932	1407253	11.44%	1.988%
29	21.604	3140	3148	3152	rBV	2365223	3893248	31.66%	5.500%
30	21.645	3152	3155	3167	rVB	326598	555350	4.52%	0.785%
31	23.892	3532	3537	3545	rBV2	147524	429321	3.49%	0.607%
32	24.933	3706	3714	3725	rBV	1552261	3928816	31.95%	5.550%

Sum of corrected areas: 70785905

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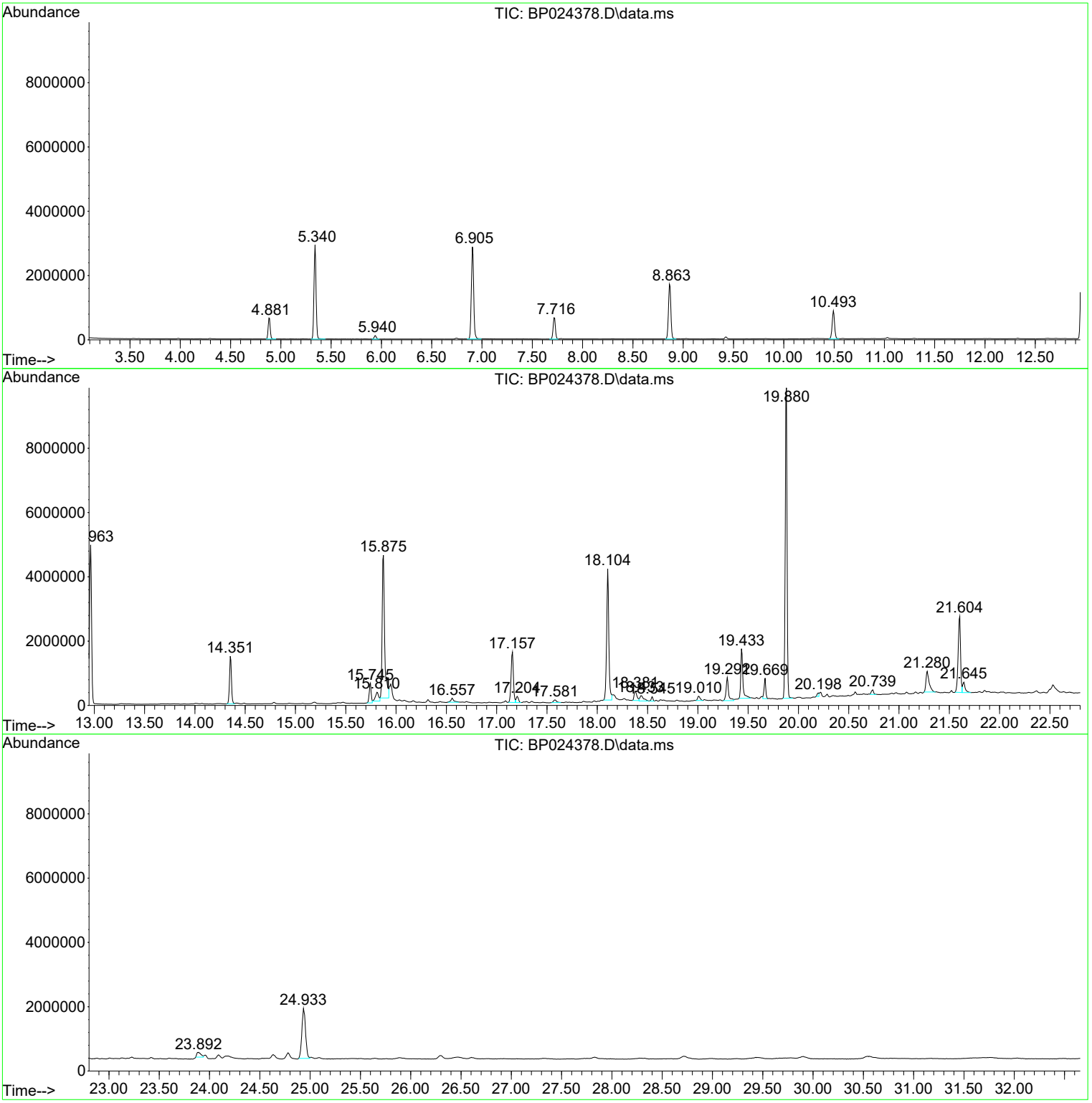
BNA_P
ClientSampleId :
PL-714-COMP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.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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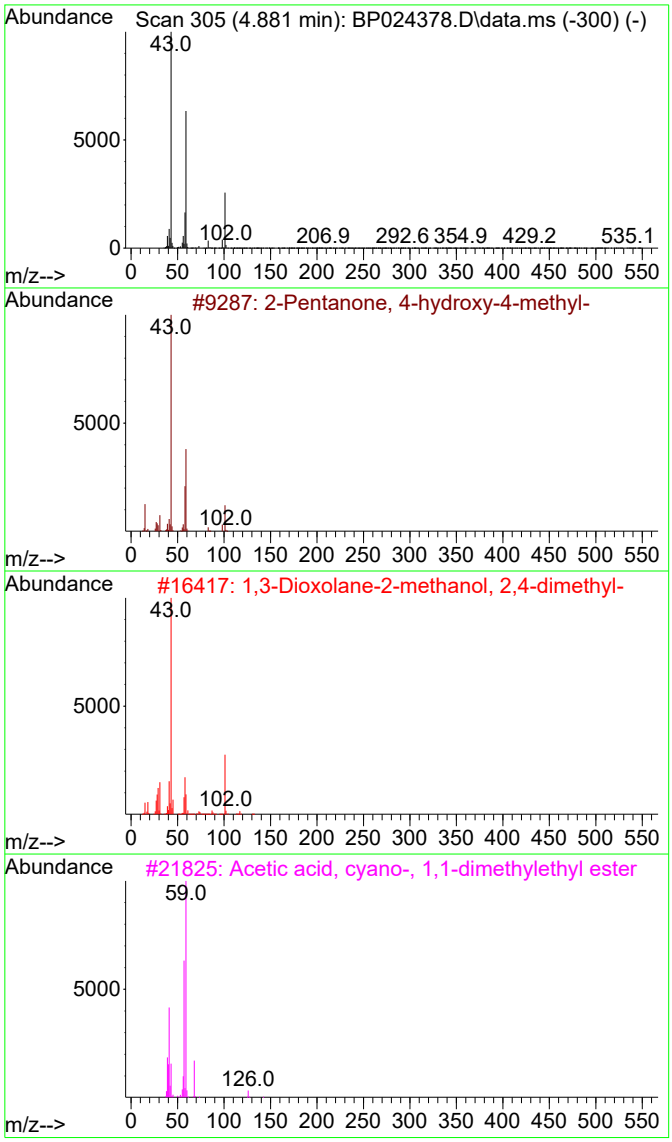
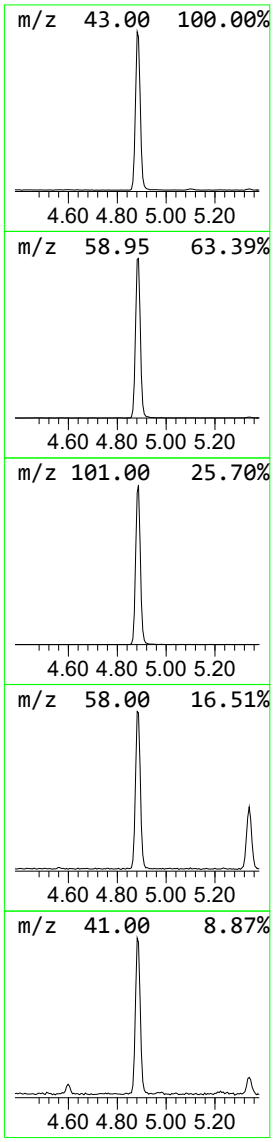
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.881	17.84 ng	914899	1,4-Dichlorobenzene-d4	7.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17





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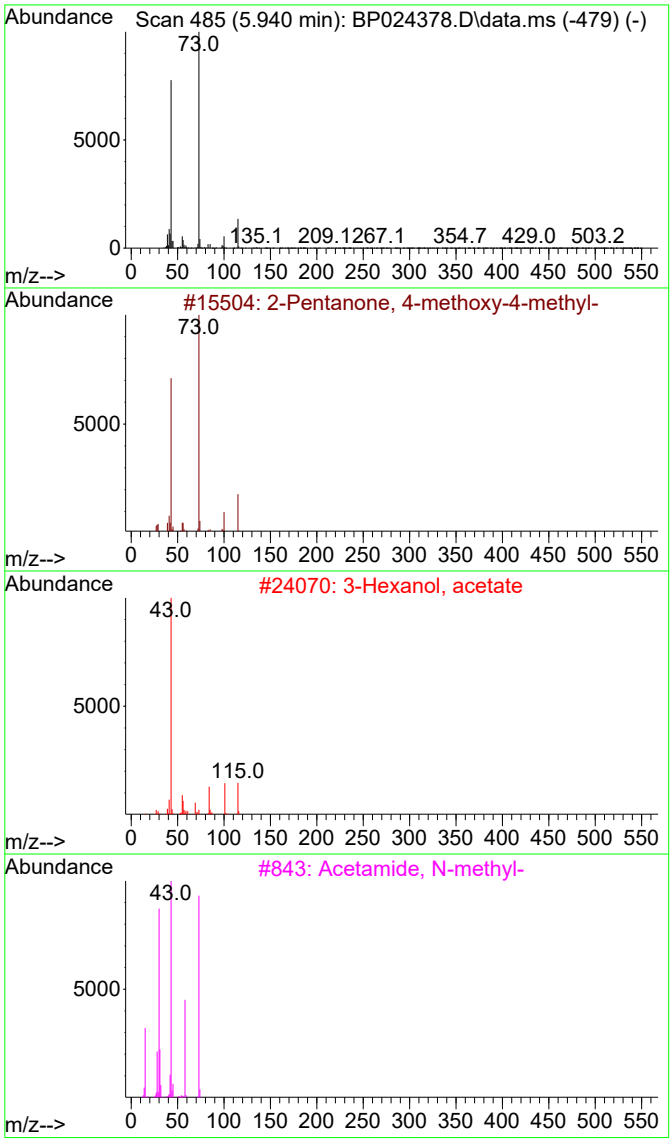
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

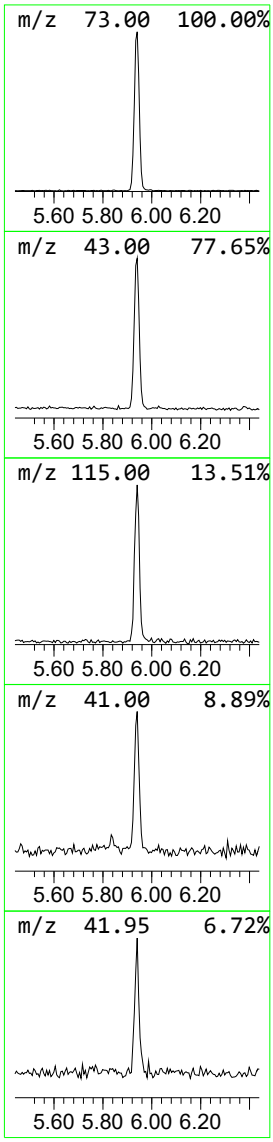
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.940	3.00 ng	153636	1,4-Dichlorobenzene-d4	7.722

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	38
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	38
4	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
5	2-Methyl-2,4-dimethoxybutane	132	C7H16O2	039836-89-0	17





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Instrument :
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ClientSampleId :
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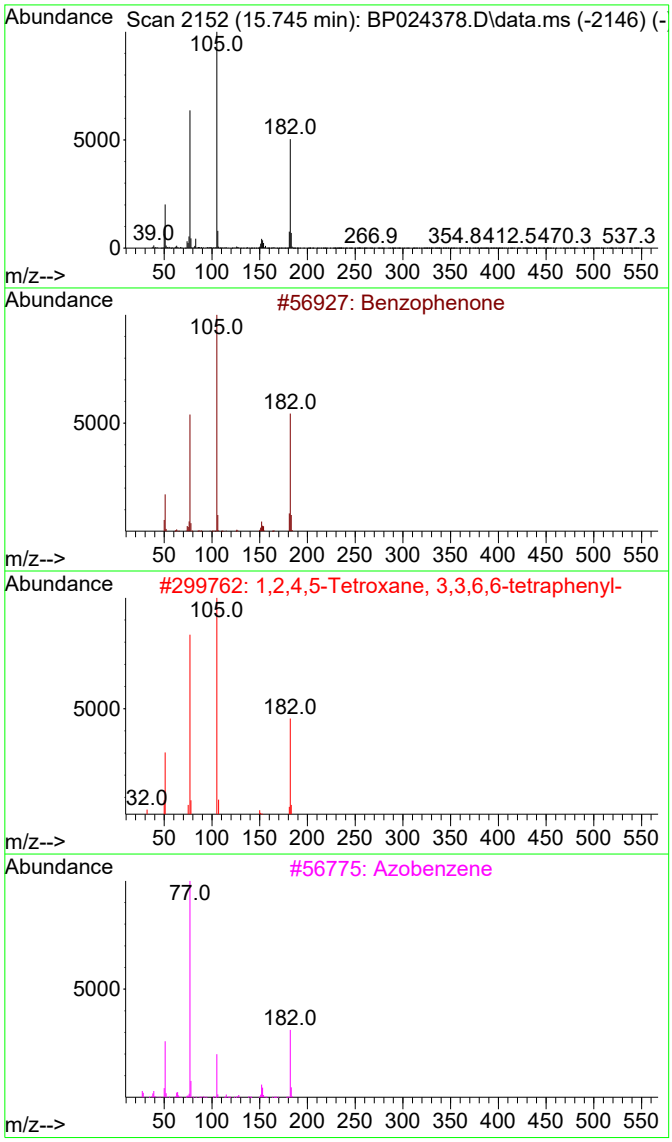
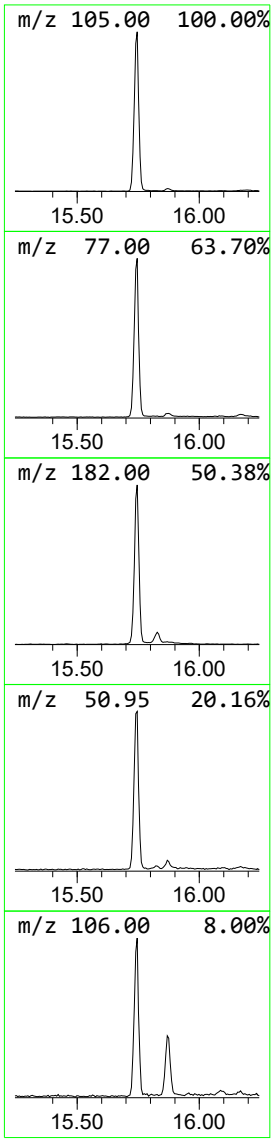
****

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	7.99 ng	807332	Acenaphthene-d10	14.351

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	Azobenzene	182	C12H10N2	000103-33-3	64
4	Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	45
5	1,1-Diphenyl-2-phenylthiobut-3-e...	332	C22H20OS	097370-20-2	36





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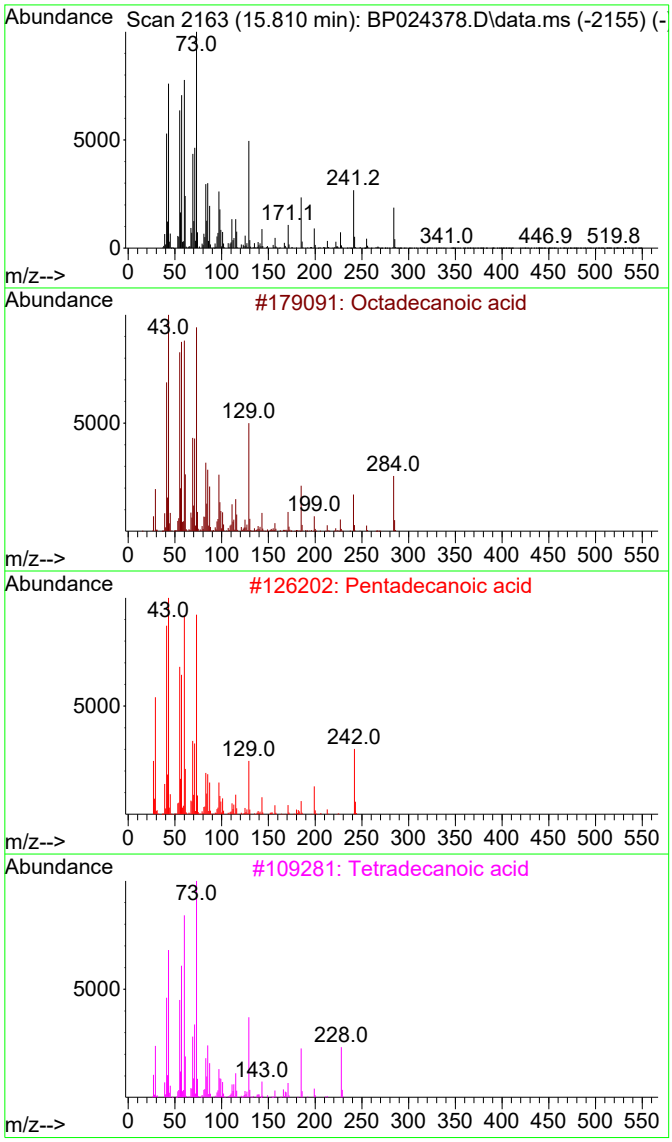
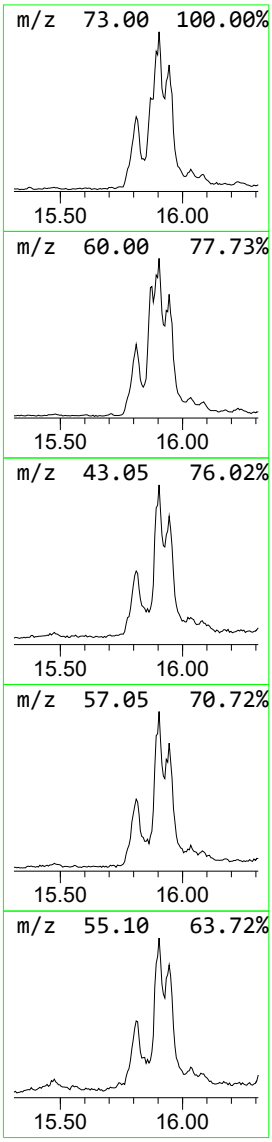
****

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.810	4.99 ng	617357	Phenanthrene-d10	17.157

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	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Operator : RC/JU
Sample : Q1842-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PL-714-COMP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
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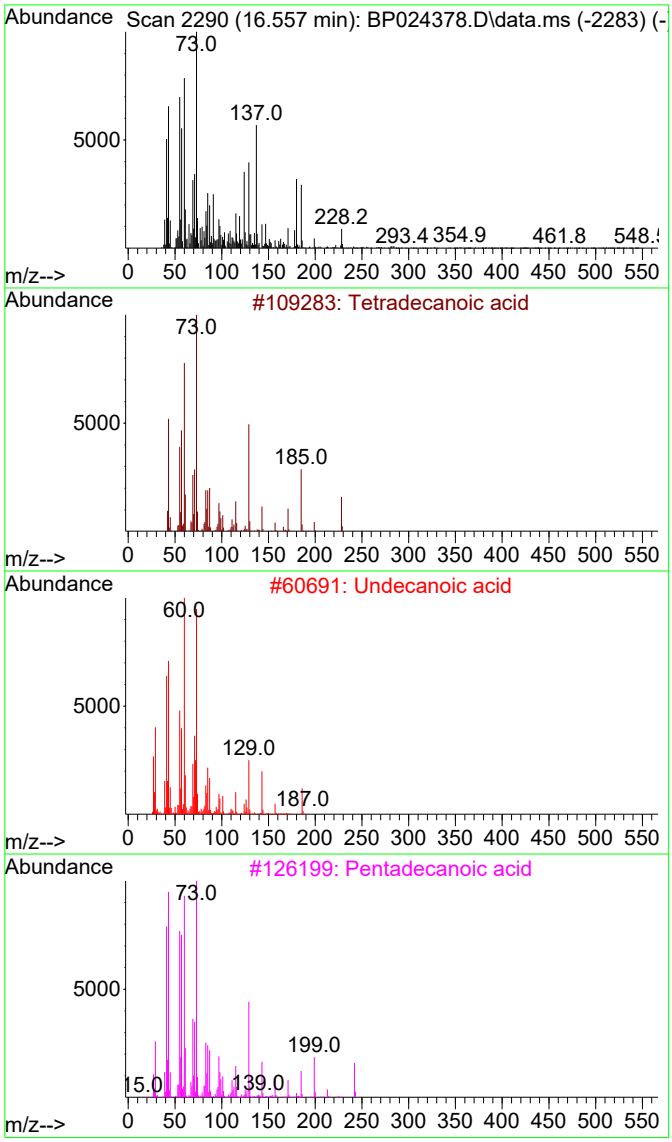
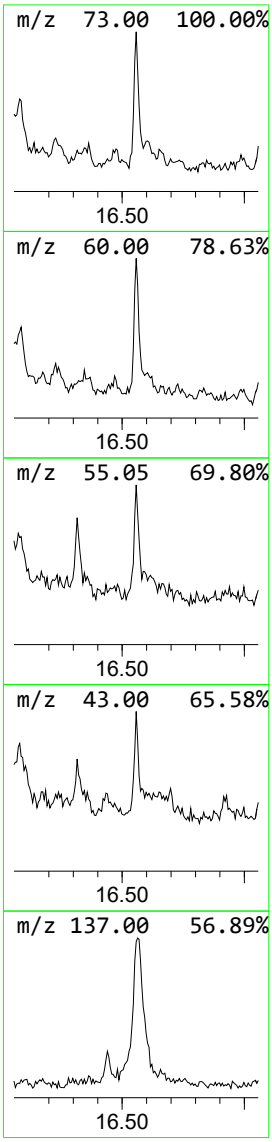
****

Peak Number 5 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.557	2.13 ng	263838	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
2	Undecanoic acid	186	C11H22O2	000112-37-8	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	Tridecanoic acid	214	C13H26O2	000638-53-9	52





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PL-714-COMP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
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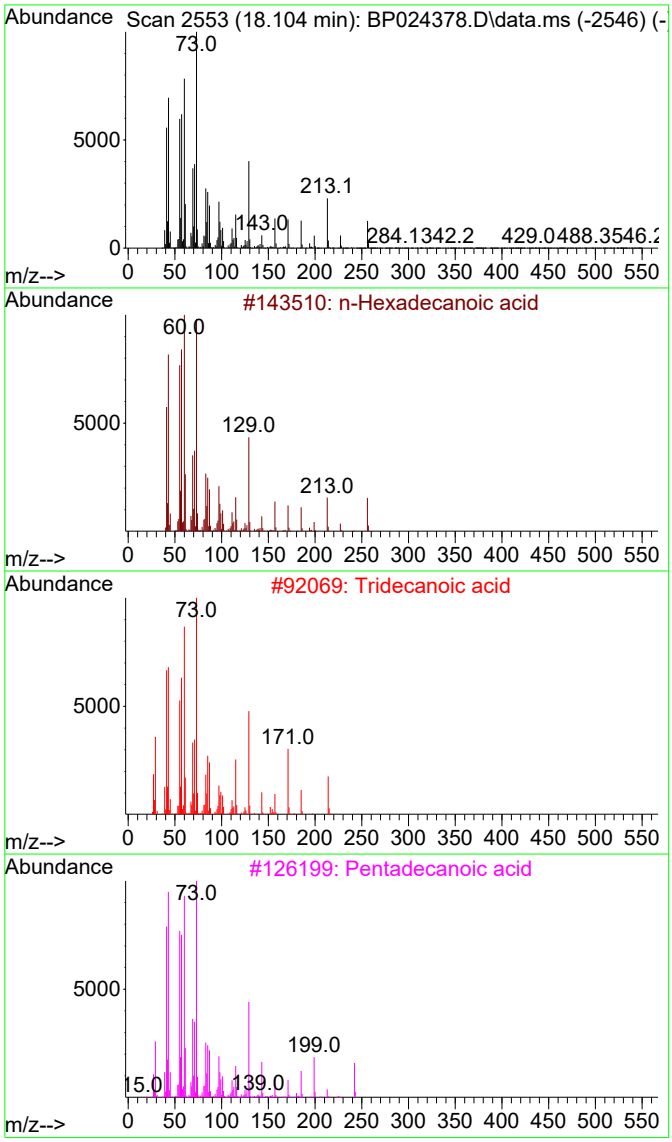
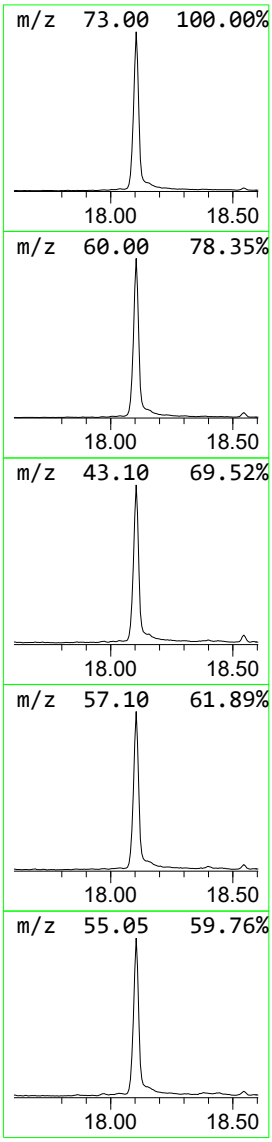
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	49.78 ng	6154810	Phenanthrene-d10	17.157

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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Sample : Q1842-13
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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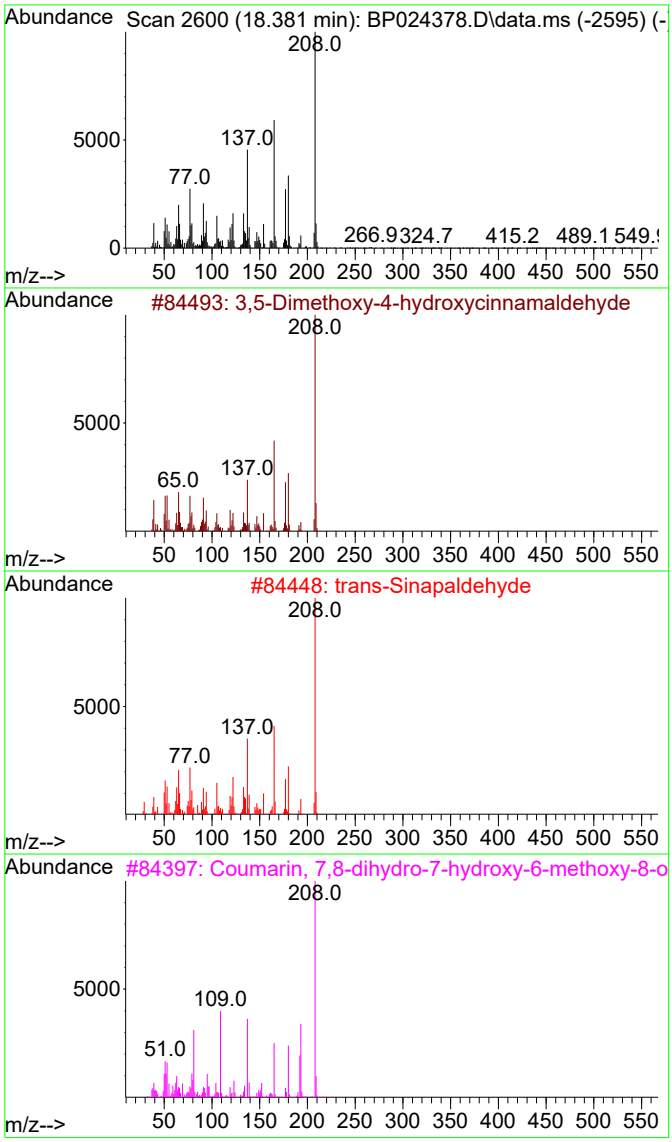
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

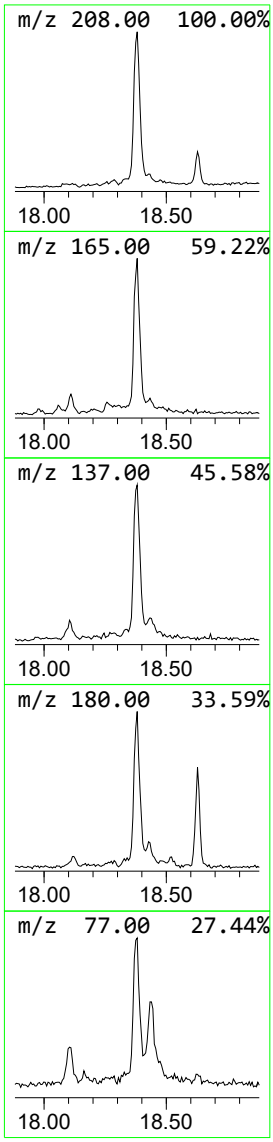
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.381	4.49 ng	554485	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	97
2	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	93
3	Coumarin, 7,8-dihydro-7-hydroxy-...	208	C10H8O5	1000263-13-6	58
4	2-Allyl-3-ethoxy-4-methoxyphenol	208	C12H16O3	1000122-70-6	58
5	Benzene, 1,2,3-trimethoxy-5-(2-p...	208	C12H16O3	000487-11-6	46





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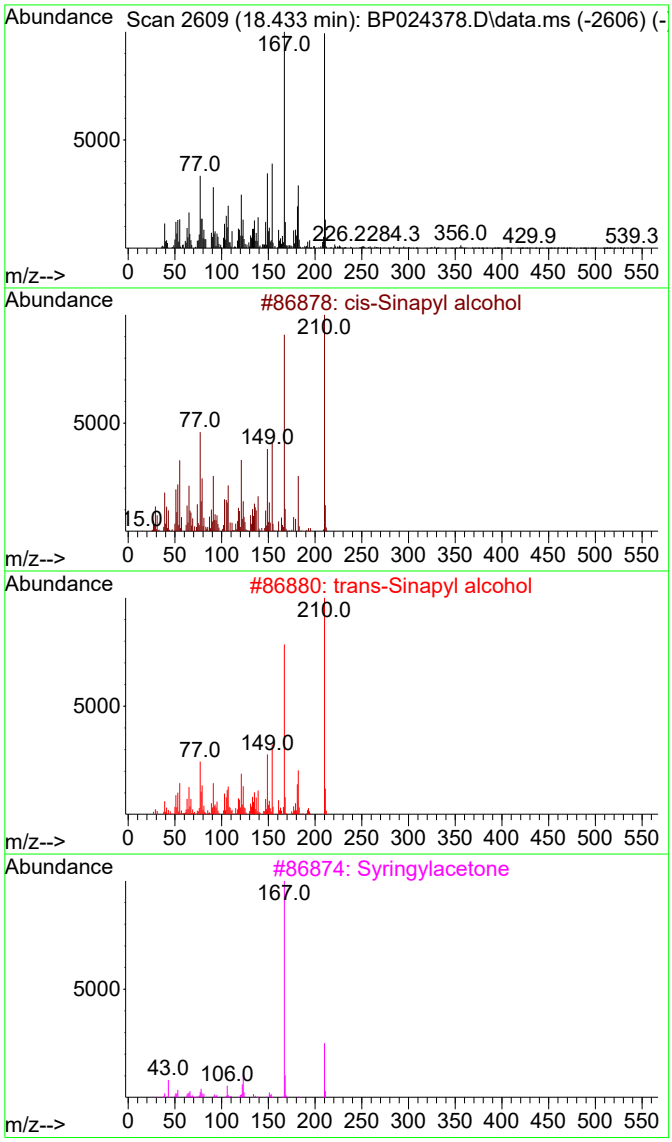
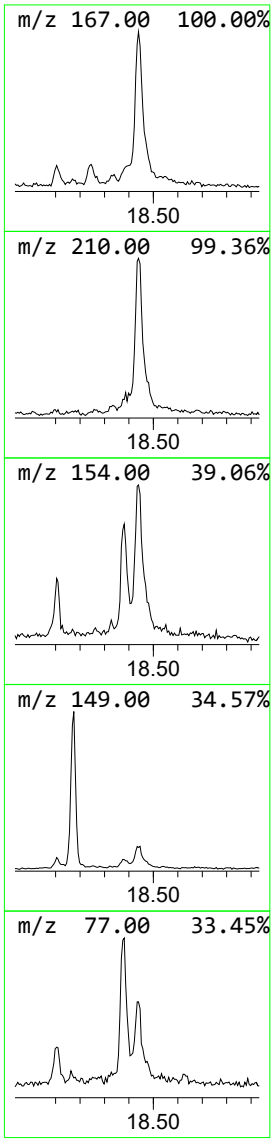
****

Peak Number 8 cis-Sinapyl alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.433	3.33 ng	411364	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	94
2	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	70
3	Syringylacetone	210	C11H14O4	019037-58-2	60
4	1-(1-Hydroxybutyl)-2,5-dimethoxy...	210	C12H18O3	149083-03-4	49
5	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	42





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TIC Library : C:\Database\NIST20.L
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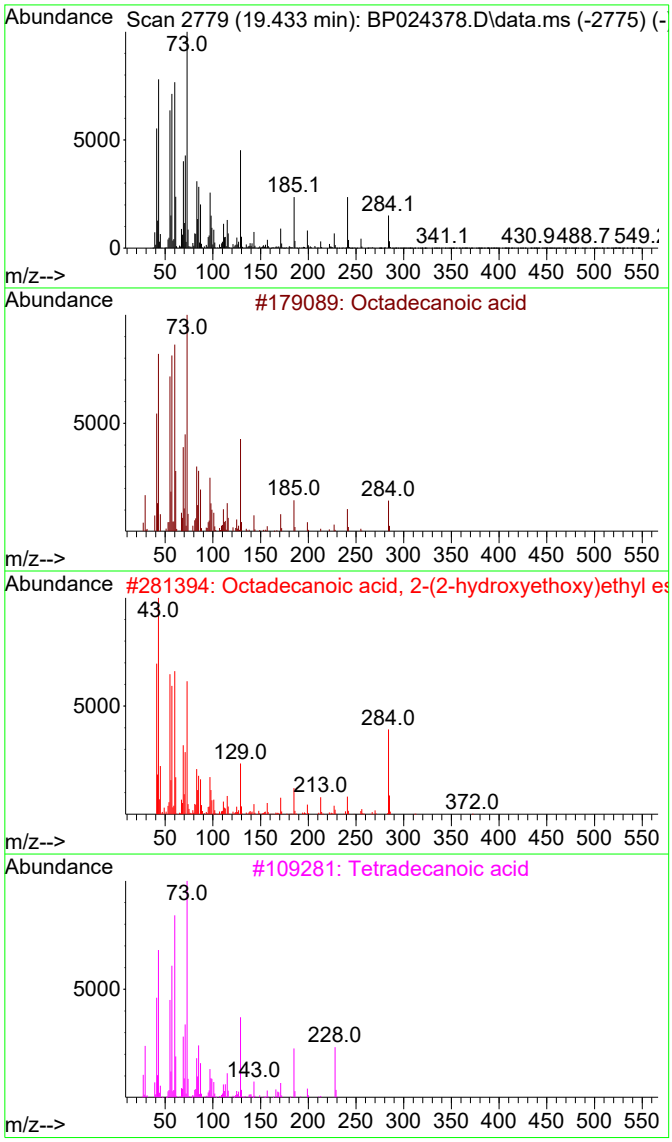
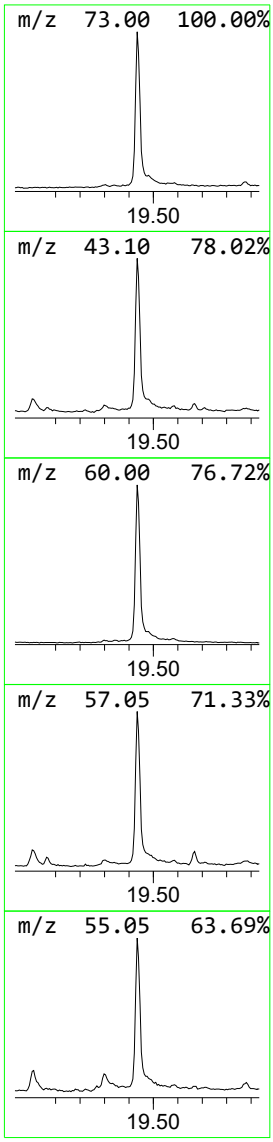
****
Peak Number 9 Octadecanoic acid, 2-(2-hyd... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	11.57 ng	2251380	Chrysene-d12	21.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042225\
Data File : BP024378.D
Acq On : 22 Apr 2025 14:41
Operator : RC/JU
Sample : Q1842-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PL-714-COMP-10

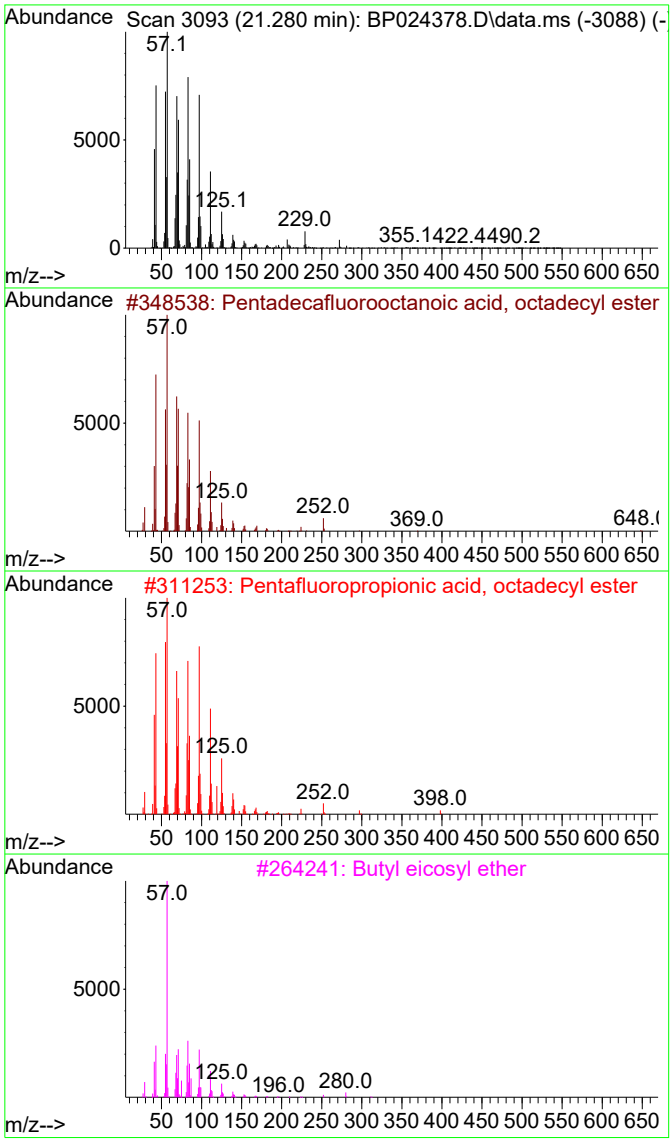
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

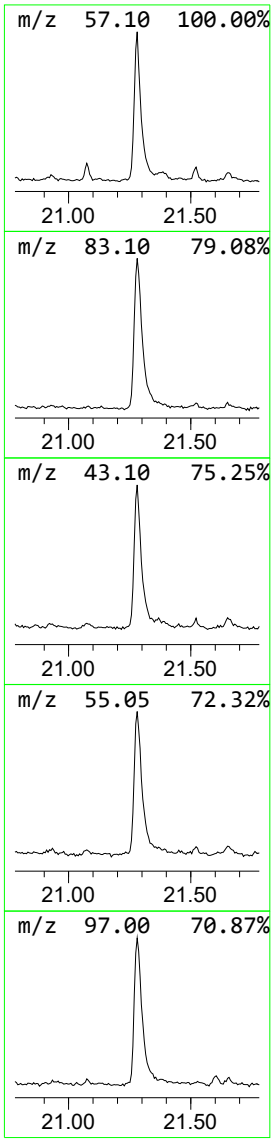
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.280	7.23 ng	1407250	Chrysene-d12	21.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
3	Butyl eicosyl ether	354	C24H50O	1000406-40-7	91
4	Butyl docosyl ether	382	C26H54O	1000406-40-8	91
5	Hexadecyl propyl ether	284	C19H40O	1000406-27-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042225\
Data File : BP024378.D
Acq On : 22 Apr 2025 14:41
Operator : RC/JU
Sample : Q1842-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PL-714-COMP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.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-...	4.881	17.8	ng	914899	1	7.722	1025810	20.0
2-Pentanone, 4-...	5.940	3.0	ng	153636	1	7.722	1025810	20.0
Benzophenone	15.745	8.0	ng	807332	3	14.351	2020830	20.0
Octadecanoic acid	15.810	5.0	ng	617357	4	17.157	2472600	20.0
Tetradecanoic acid	16.557	2.1	ng	263838	4	17.157	2472600	20.0
n-Hexadecanoic ...	18.104	49.8	ng	6154810	4	17.157	2472600	20.0
3,5-Dimethoxy-4...	18.381	4.5	ng	554485	4	17.157	2472600	20.0
cis-Sinapyl alc...	18.433	3.3	ng	411364	4	17.157	2472600	20.0
Octadecanoic ac...	19.433	11.6	ng	2251380	5	21.604	3893250	20.0
Pentadecafluoro...	21.280	7.2	ng	1407250	5	21.604	3893250	20.0