LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042825\
Data File : BP024442.D
Acq On : 28 Apr 2025 18:24
Operator : RC/JU
Sample : Q1889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-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_P\Methods\8270E-BP041425.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024442.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.405	49	54	62	rVB	148123	174923	1.61%	0.325%
2	3.517	69	73	84	rBV	100602	150438	1.39%	0.279%
3	4.881	298	305	316	rBV	255185	361849	3.34%	0.672%
4	5.340	376	383	397	rBV	2693248	3979251	36.69%	7.392%
5	6.905	639	649	670	rBV	2657385	4246581	39.16%	7.889%
6	7.716	780	787	795	rBV	559314	852596	7.86%	1.584%
7	8.863	974	982	995	rBV	1736090	2755798	25.41%	5.119%
8	10.487	1250	1258	1268	rBV	705545	1194195	11.01%	2.218%
9	12.957	1669	1678	1696	rBV	4481167	6592124	60.79%	12.246%
10	14.345	1907	1914	1925	rBV	1181623	1646808	15.19%	3.059%
11	15.728	2143	2149	2156	rBV	580825	820561	7.57%	1.524%
12	15.869	2165	2173	2196	rBV	4821641	6951419	64.10%	12.913%
13	17.145	2383	2390	2404	rBV2	1310785	2042874	18.84%	3.795%
14	17.563	2455	2461	2471	rBV2	68859	159033	1.47%	0.295%
15	18.092	2544	2551	2567	rBV	720071	1275082	11.76%	2.369%
16	18.533	2621	2626	2631	rBV	175142	209839	1.93%	0.390%
17	19.339	2752	2763	2772	rBV	877786	2045670	18.86%	3.800%
18	19.422	2772	2777	2796	rVB	462582	844995	7.79%	1.570%
19	19.875	2847	2854	2863	rBV	8202962	10844585	100.00%	20.145%
20	20.445	2948	2951	2956	rBV	89413	137269	1.27%	0.255%
21	21.257	3084	3089	3101	rBV	335497	751759	6.93%	1.396%
22	21.586	3139	3145	3153	rBV	1623854	2471502	22.79%	4.591%
23	23.180	3410	3416	3428	rVB3	207617	498377	4.60%	0.926%
24	24.927	3705	3713	3728	rVB	965900	2824603	26.05%	5.247%

Sum of corrected areas: 53832131

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042825\
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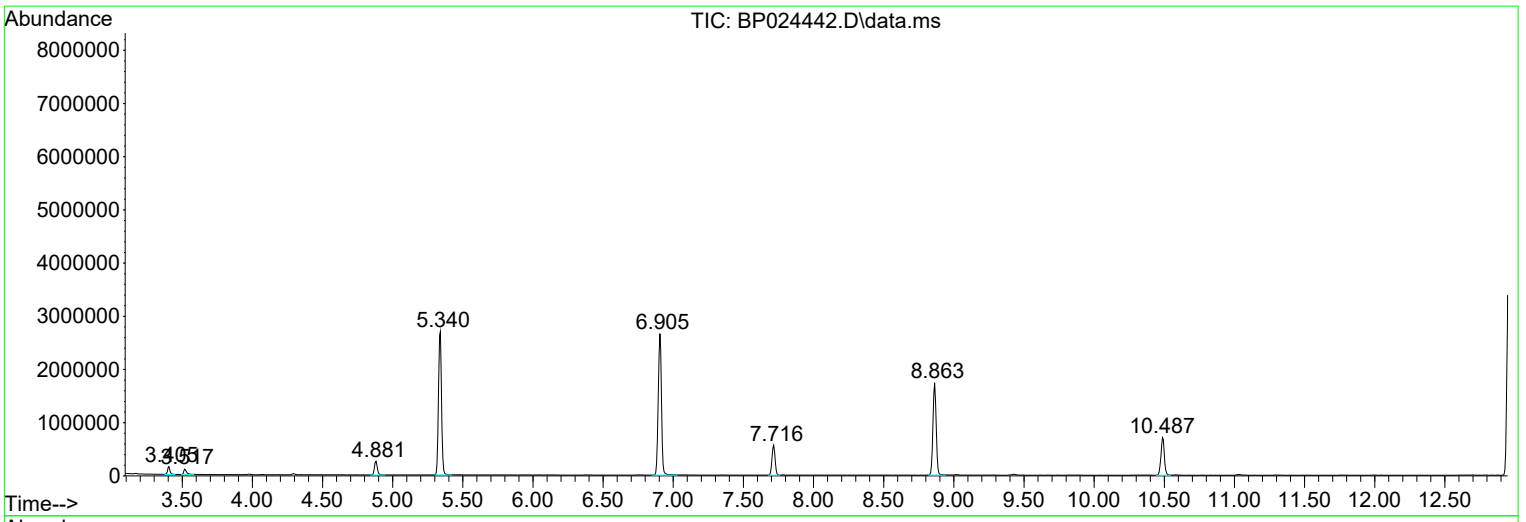
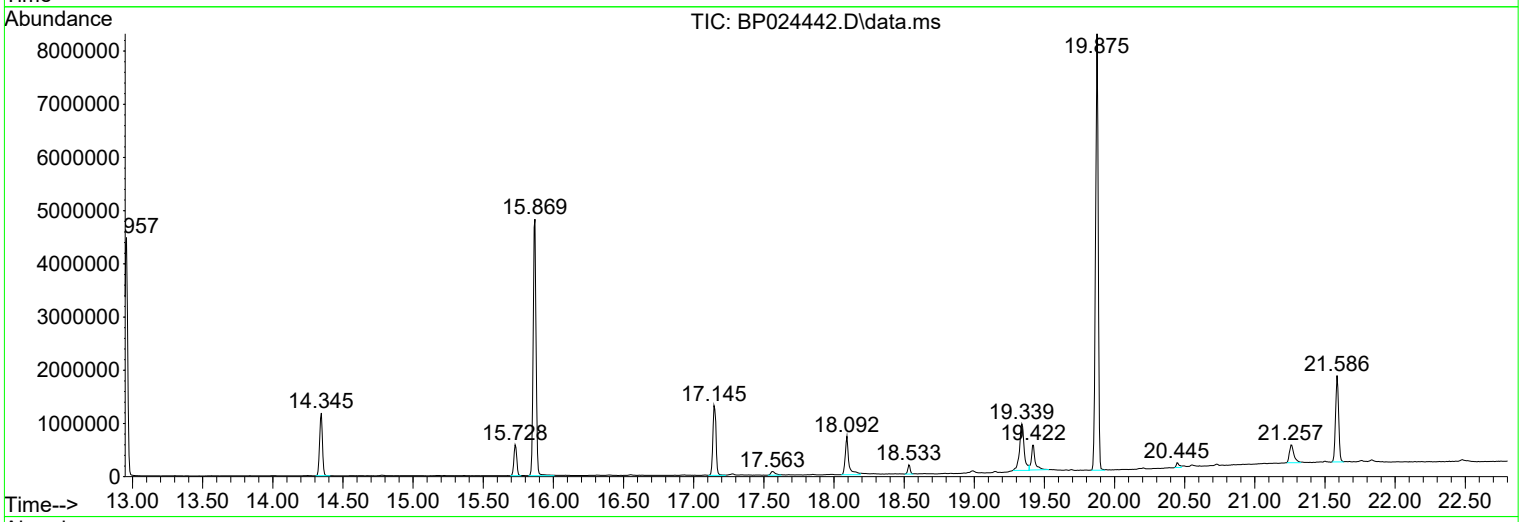
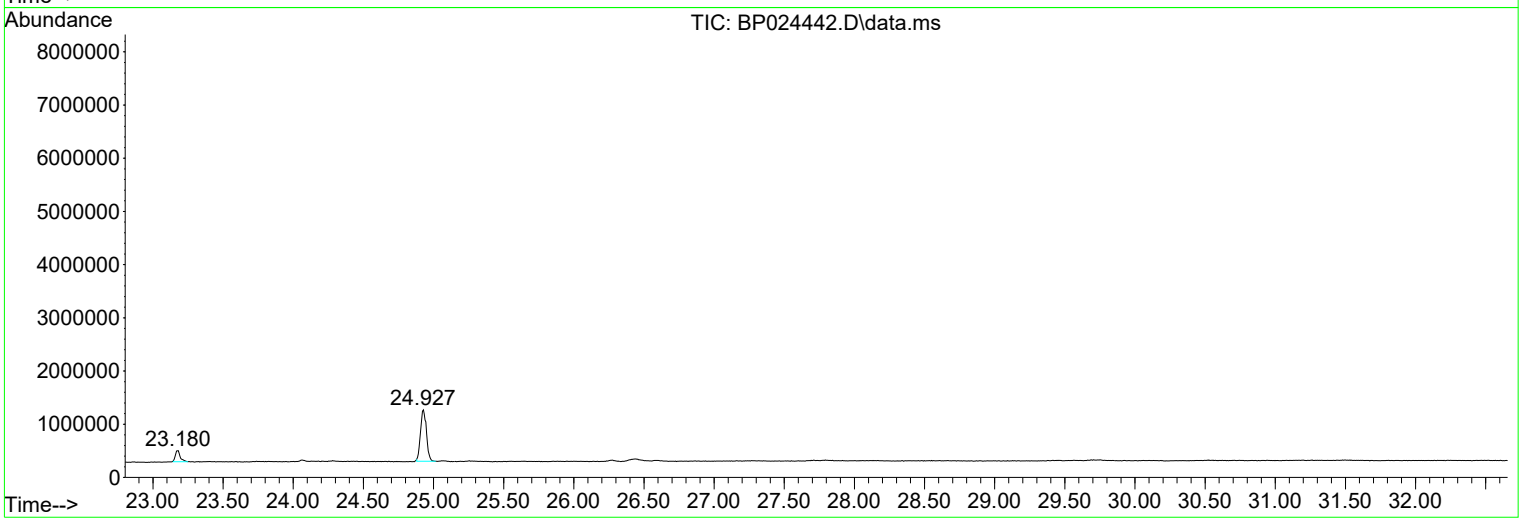
Instrument :
BNA_P
ClientSampleId :
COMP-3

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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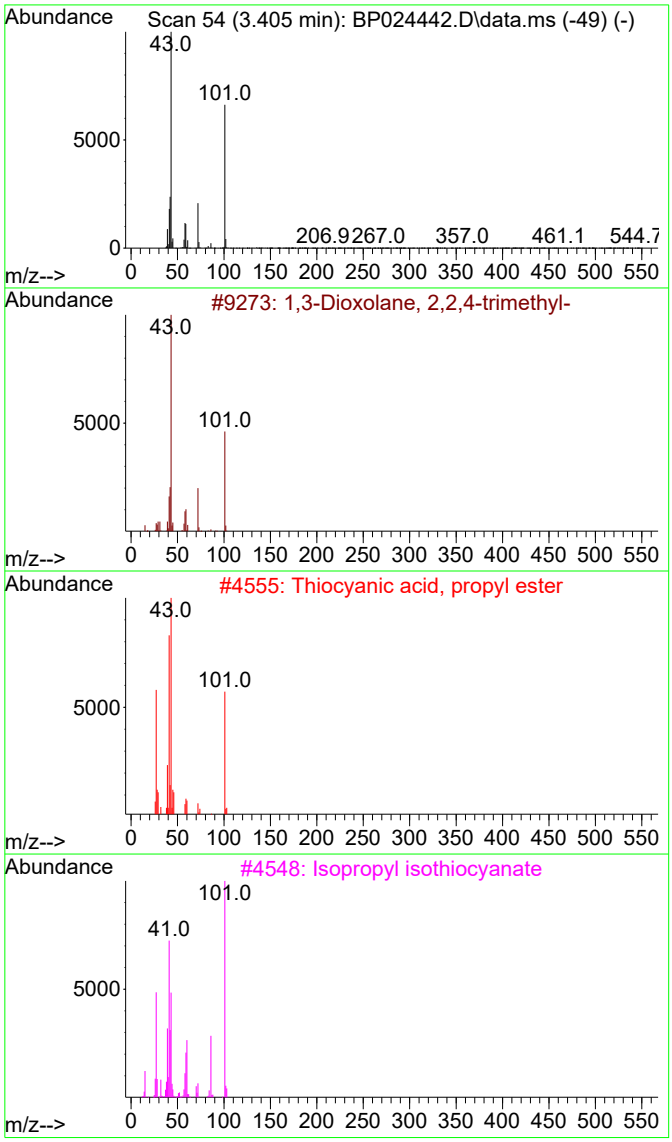
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

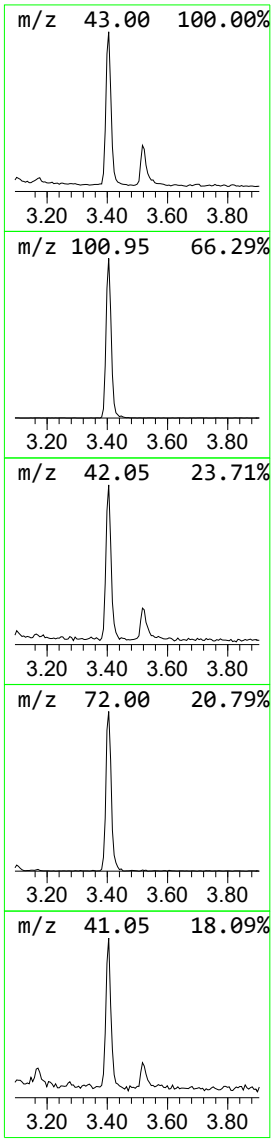
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.405	4.10 ng	174923	1,4-Dichlorobenzene-d4	7.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	53
3	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	50
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	50
5	2-Pyrrolidinethione	101	C4H7NS	002295-35-4	47





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Operator : RC/JU
Sample : Q1889-03
Misc :
ALS Vial : 9 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

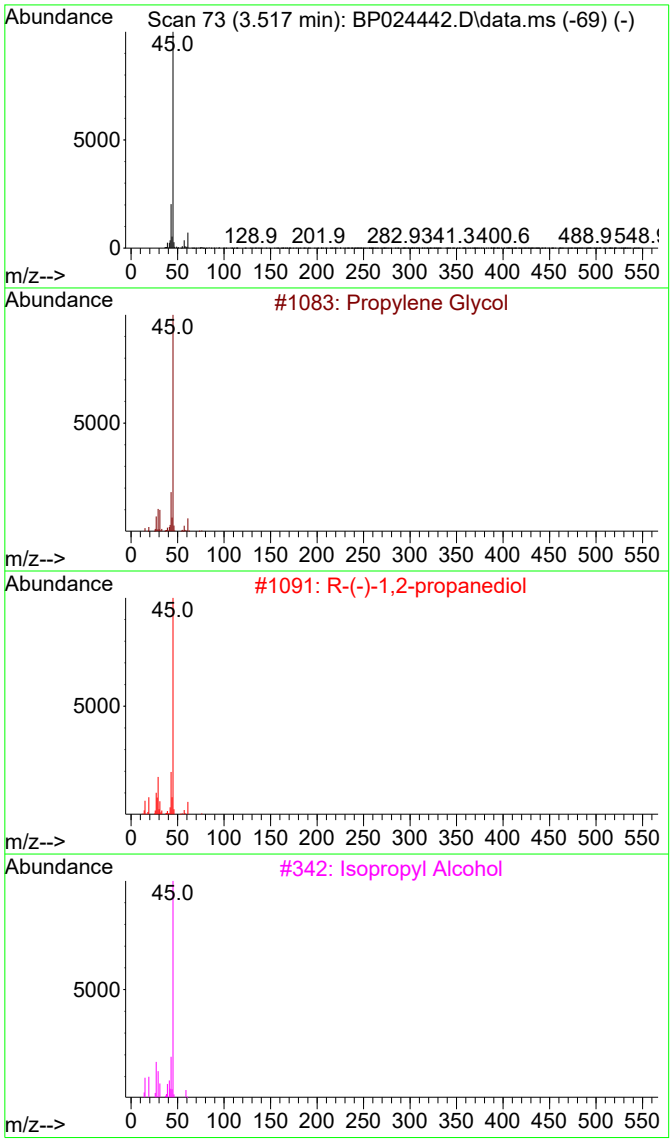
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

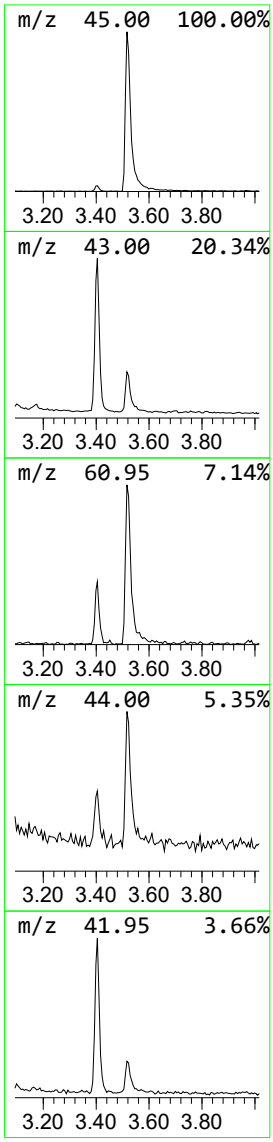
****

Peak Number 2 Propylene Glycol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.517	3.53 ng	150438	1,4-Dichlorobenzene-d4	7.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40





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Sample : Q1889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

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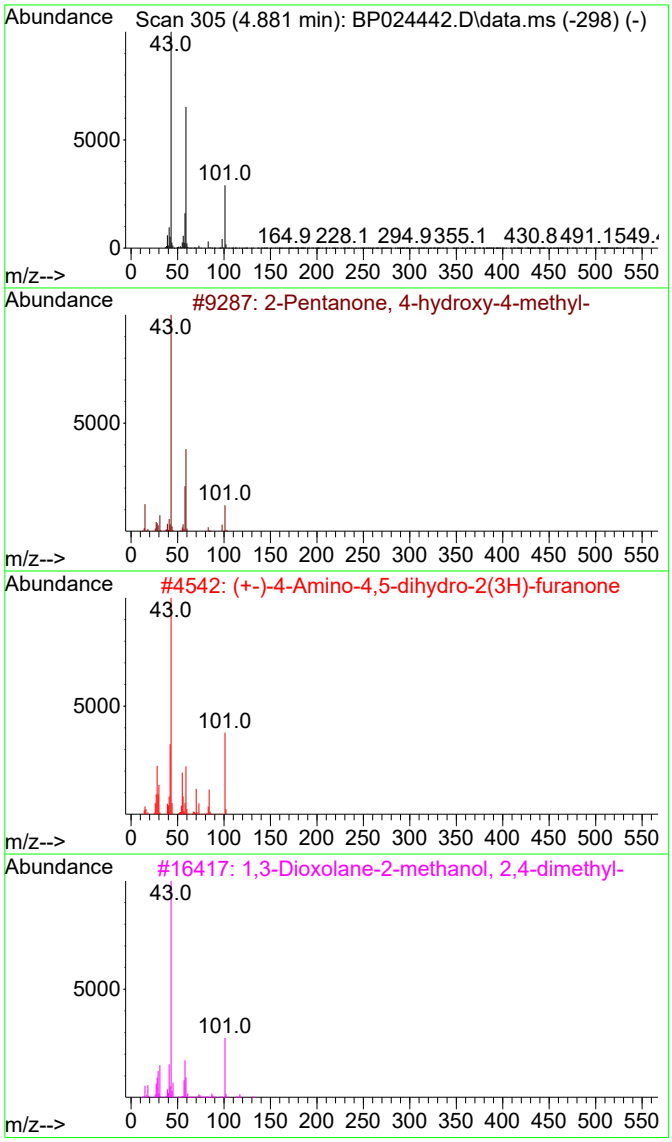
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

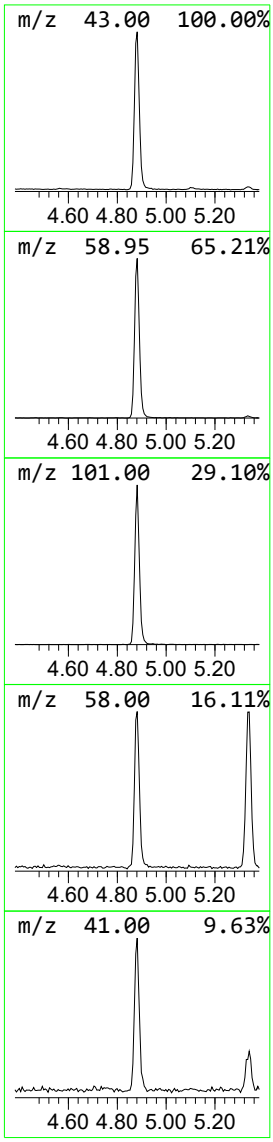
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.881	8.49 ng	361849	1,4-Dichlorobenzene-d4	7.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Instrument :
BNA_P
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TIC Library : C:\Database\NIST20.L
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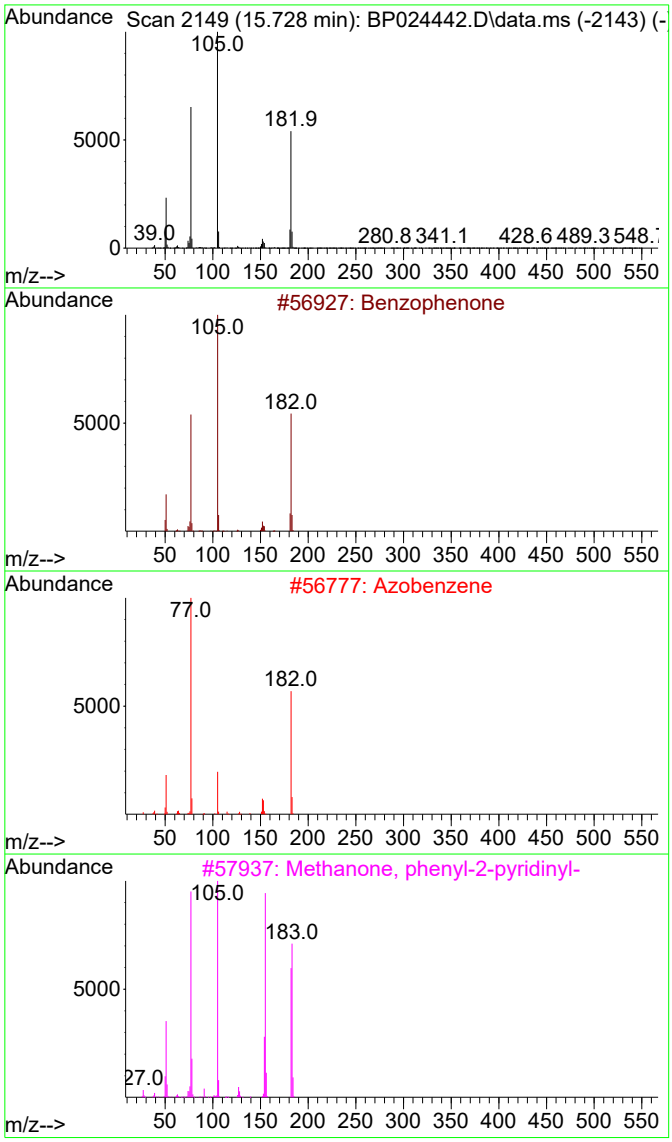
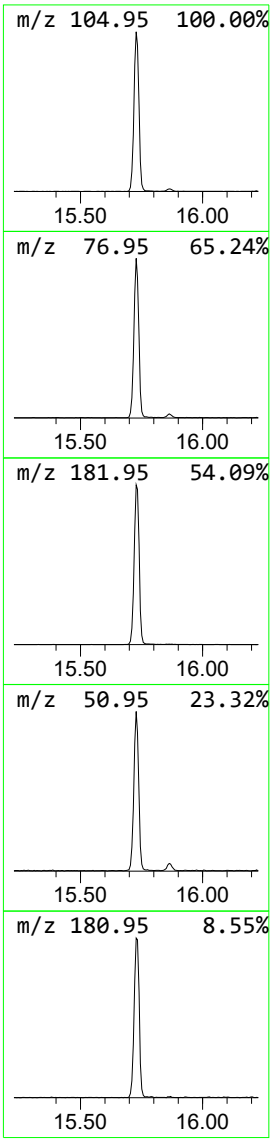
Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.728	9.97 ng	820561	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50
4	Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	45
5	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	40





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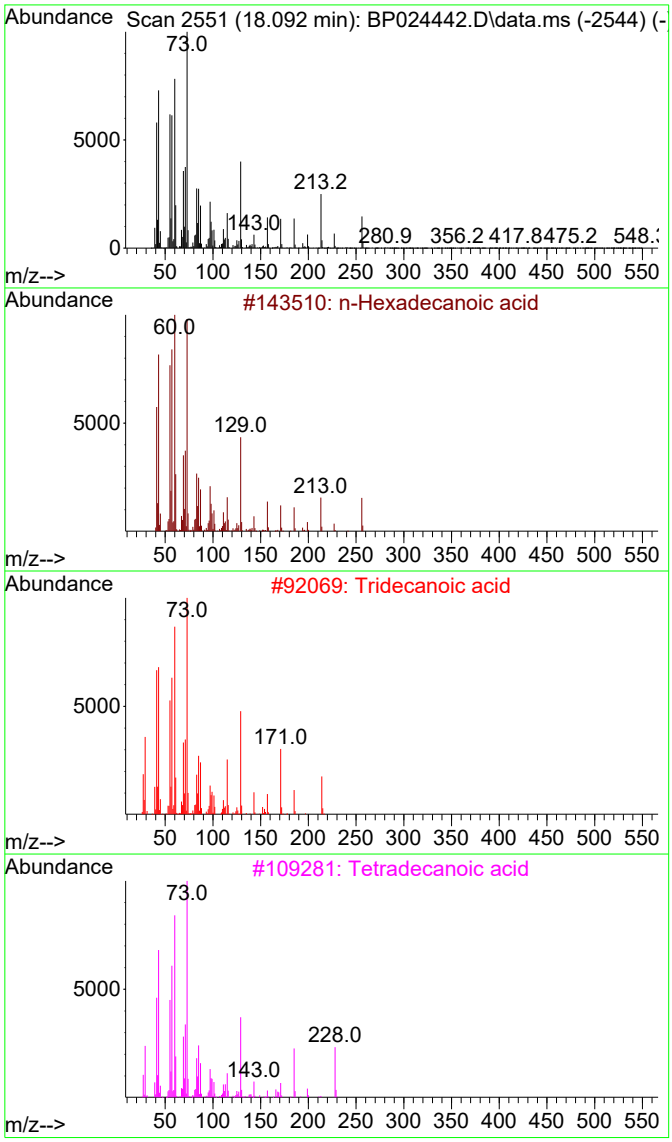
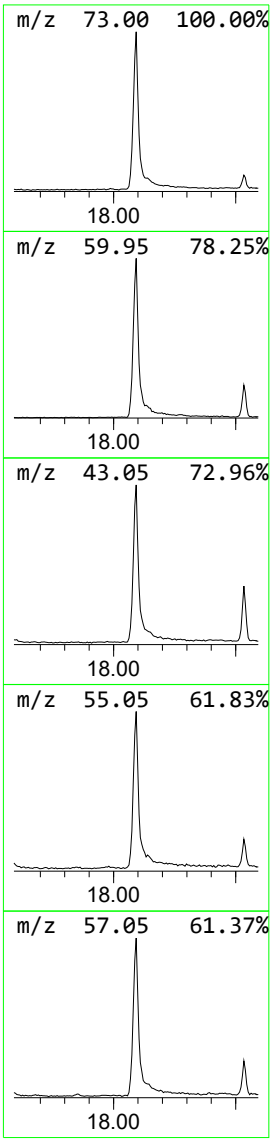
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	12.48 ng	1275080	Phenanthrene-d10	17.145

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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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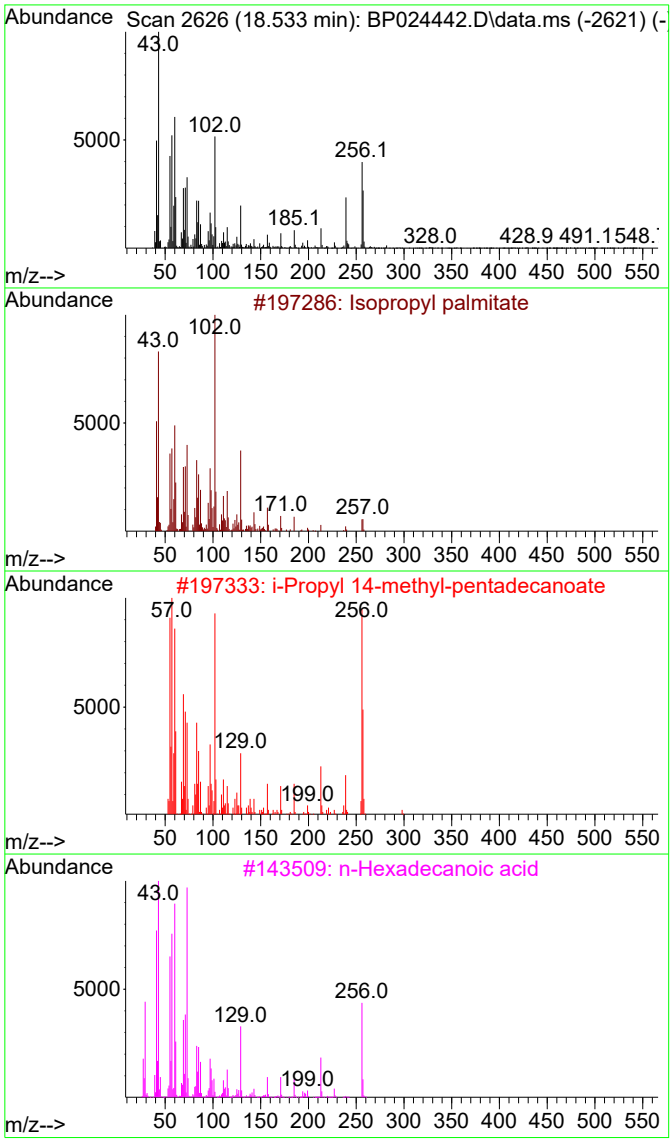
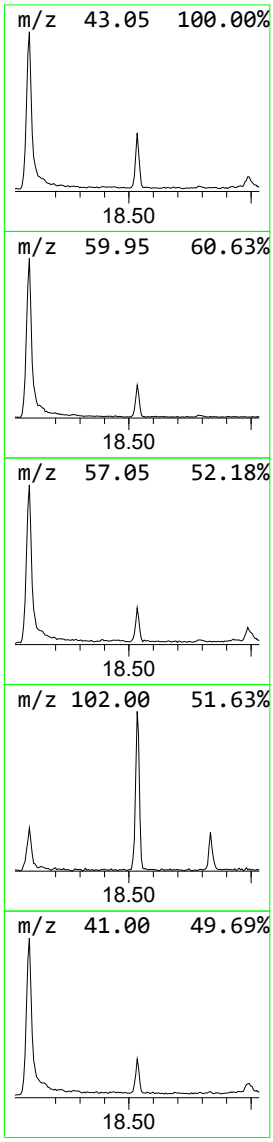
****

Peak Number 6 Isopropyl palmitate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.533	2.05 ng	209839	Phenanthrene-d10	17.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	83
2	i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	47
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	41
4	8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	38
5	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	15





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Instrument :
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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
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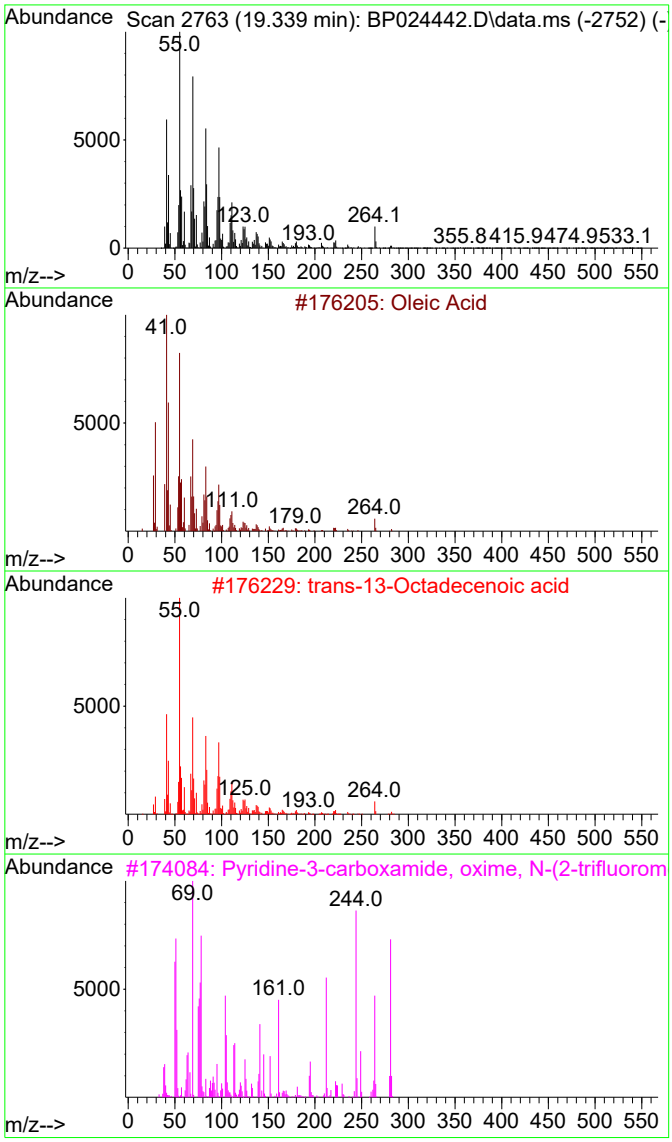
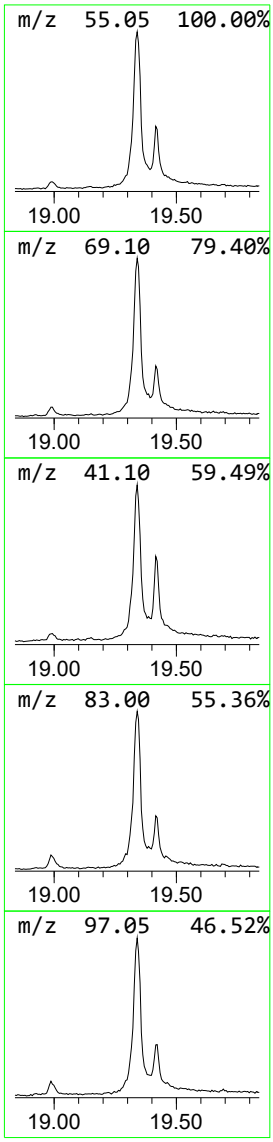
****

Peak Number 7 Oleic Acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	20.03 ng	2045670	Phenanthrene-d10	17.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	99
2	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	95
3	Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	93
4	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	91
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	89





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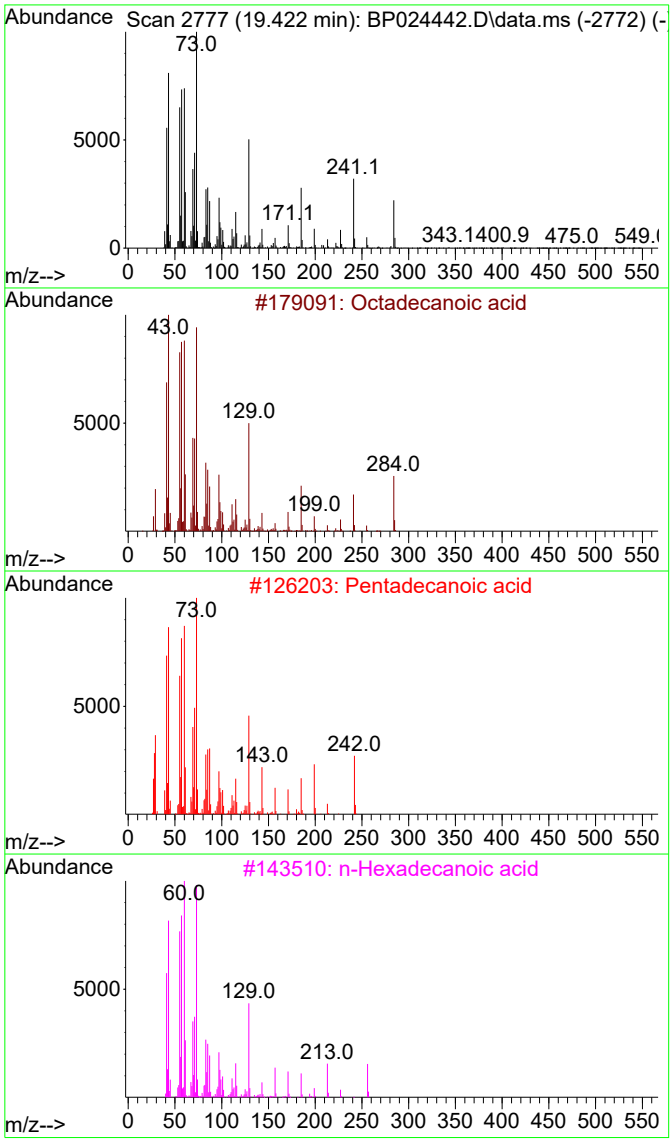
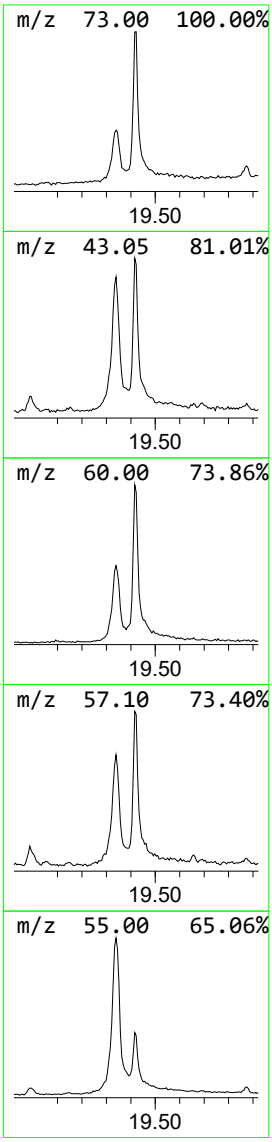
Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	6.84 ng	844995	Chrysene-d12	21.586

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	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Instrument :
BNA_P
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

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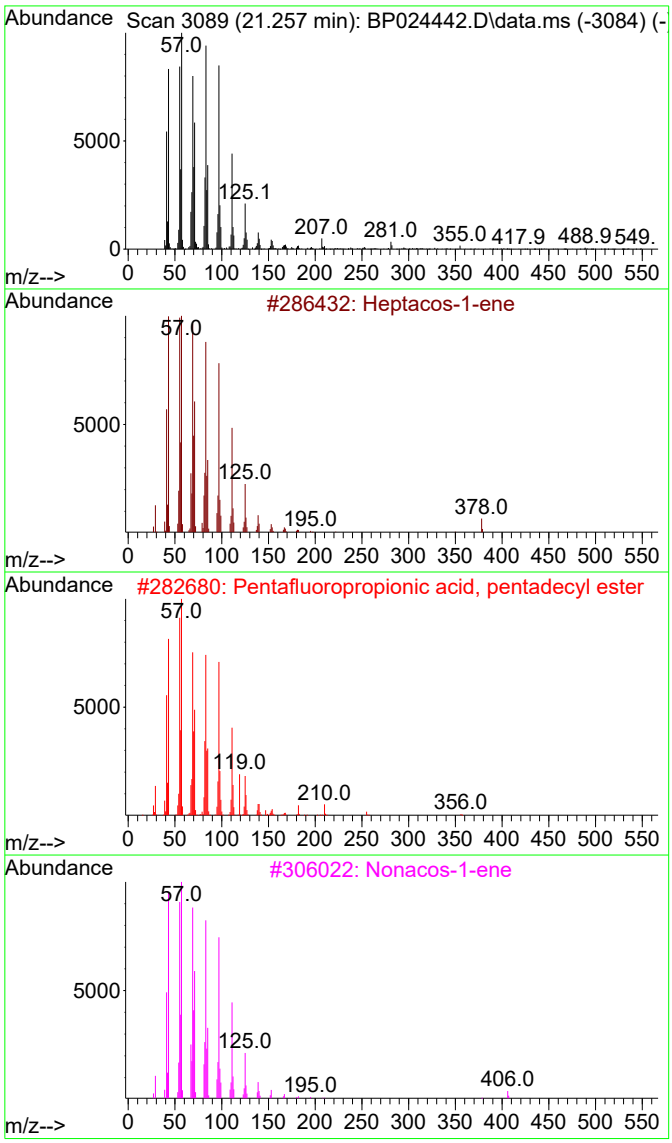
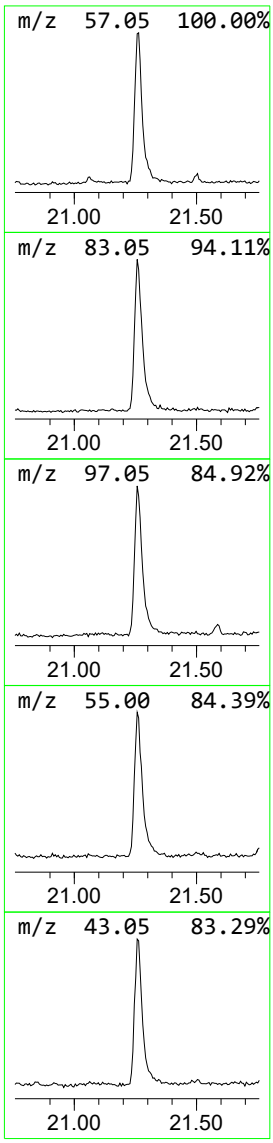
Peak Number 9 Heptacos-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	6.08 ng	751759	Chrysene-d12	21.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacos-1-ene	378	C27H54	015306-27-1	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Nonacos-1-ene	406	C29H58	018835-35-3	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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Acq On : 28 Apr 2025 18:24
Operator : RC/JU
Sample : Q1889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-3

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

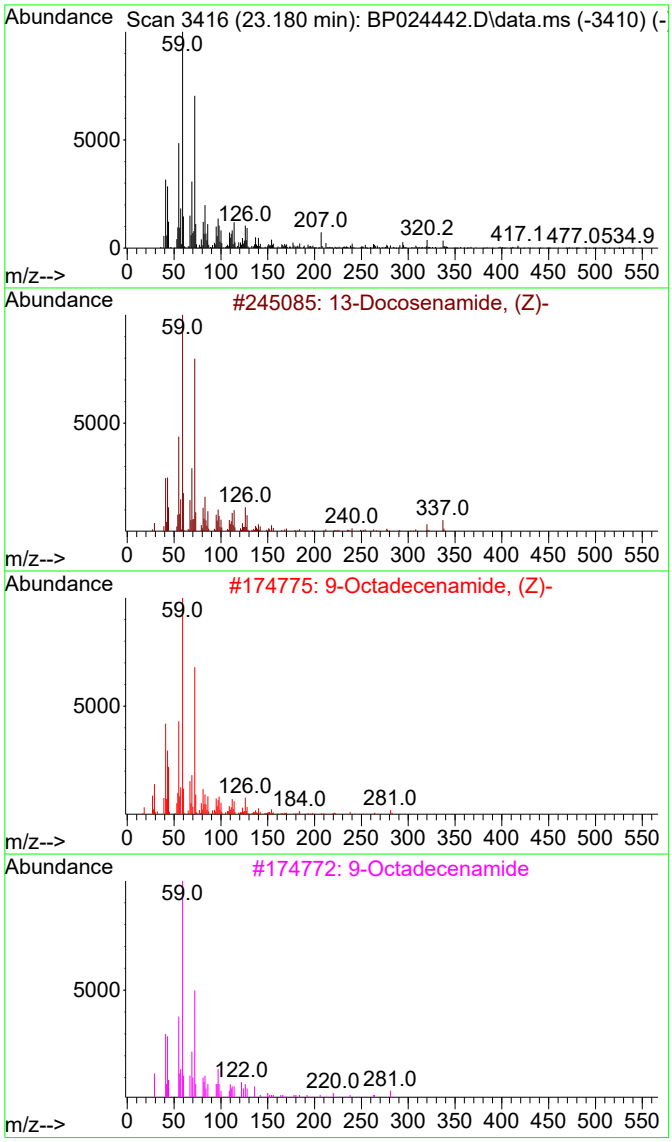
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

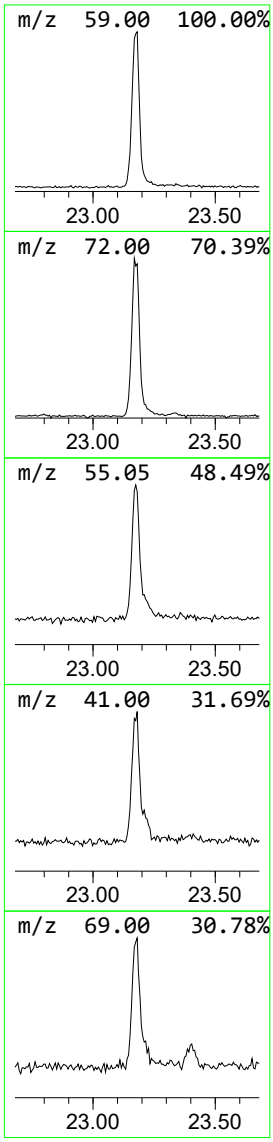
****

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.180	4.03 ng	498377	Chrysene-d12	21.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	99
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
3	9-Octadecenamide	281	C18H35NO	003322-62-1	72
4	Tetradecanamide	227	C14H29NO	000638-58-4	72
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042825\
Data File : BP024442.D
Acq On : 28 Apr 2025 18:24
Operator : RC/JU
Sample : Q1889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-3

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
1,3-Dioxolane, ...	3.405	4.1	ng	174923	1	7.716	852596	20.0
Propylene Glycol	3.517	3.5	ng	150438	1	7.716	852596	20.0
2-Pentanone, 4-...	4.881	8.5	ng	361849	1	7.716	852596	20.0
Benzophenone	15.728	10.0	ng	820561	3	14.345	1646810	20.0
n-Hexadecanoic ...	18.092	12.5	ng	1275080	4	17.145	2042870	20.0
Isopropyl palmi...	18.533	2.0	ng	209839	4	17.145	2042870	20.0
Oleic Acid	19.339	20.0	ng	2045670	4	17.145	2042870	20.0
Octadecanoic acid	19.422	6.8	ng	844995	5	21.586	2471500	20.0
Heptacos-1-ene	21.257	6.1	ng	751759	5	21.586	2471500	20.0
13-Docosenamide...	23.180	4.0	ng	498377	5	21.586	2471500	20.0